INTERACTION ENERGIES, LATTICES, AND DESIGNS

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INTERACTION ENERGIES, LATTICES, AND DESIGNS

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To my teachers.

PREFACE

This thesis has four chapters. The first three concern the location of mass on spheres or projective space, to minimize energies. For the Columb potential on the unit sphere, this is a classical problem, related to arranging electrons to minimize their energy. Restricting our potentials to be polynomials in the squared distance between points, we show in the Chapter 1 that there exist discrete minimal energy distributions. In addition we pose a conjecture on discreteness of minimizers for another class of energies while showing these minimizers must have empty interior.

In Chapter 2, we discover that highly symmetric distributions of points minimize energies over probability measures for potentials which are completely monotonic up to some degree, guided by the work of H. Cohn and A. Kumar. We make conjectures about optima for a class of energies calculated by summing absolute values of inner products raised to a positive power. Through reformulation, these observations give rise to new mixed-volume inequalities and conjectures. Our numerical experiments also lead to discovery of a new highly symmetric complex projective design which we detail the construction for. In this chapter we also provide details on a computer assisted argument which shows optimality of the 600-cell for such energies (via interval arithmetic).

In Chapter 3 we also investigate energies having minimizers with a small number of distinct inner products. We focus here on discrete energies, confirming that for small p the repeated orthonormal basis minimizes the ℓ_p-norm of the inner products out of all unit norm configurations. These results have analogs for simplices which we also prove.

Finally, the topics in Chapter 4 differ substantially from the first three. Here we show that real tight frames that generate lattices must be rational, and that the same holds for other vector systems with structured matrices of outer products. We describe a construction of lattices from distance transitive graphs which gives rise to strongly eutactic lattices. We discuss properties of this construction and also detail potential applications of lattices generated by incoherent systems of vectors.

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CHAPTER 1

ENERGY ON SPHERES AND DISCRETENESS OF MINIMIZING MEASURES

1.1 Introduction

Energy minimization on the sphere arises naturally in numerous contexts in mathematical physics, discrete and metric geometry, coding theory, signal processing, and other fields of mathematics. Many problems can be reformulated in terms of minimization of the *discrete energy*

$$E_f(\mathcal{C}) = \frac{1}{|\mathcal{C}|^2} \sum_{x,y\in\mathcal{C}} f(\langle x, y\rangle) \tag{1.1.1}$$

over all N-point configurations $\mathcal{C} \subset \mathbb{S}^{d-1}$, or of the continuous *energy integral*

$$I_f(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y\rangle) d\mu(x) d\mu(y) \tag{1.1.2}$$

over $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$, the set of all Borel probability measures. In this work, we mostly concentrate on the energy integrals. We assume that the measurable function $f : [-1, 1] \to \mathbb{R}$ is bounded below, hence the integral (1.1.2) is well defined, although it may be infinite for some measures.

Loosely speaking, minimizing the discrete N-point energy may be interpreted as finding the equilibrium position of N “particles” on the sphere, which interact according to the potential f, which depends on the distance between x and y, while minimizing the energy integral corresponds to finding the optimal distribution of unit charge on $\mathbb{S}^{d-1}$ under the same interaction. From the minimizers of energy integrals we learn the limiting behavior of the discrete problem as the number of points N goes to infinity. Observe that the interaction depends only on the distance between x and y, hence the energy (1.1.2) is invariant under orthogonal transformations.

The definitions of the discrete (1.1.1) and continuous (1.1.2) energies are compatible in the sense that

$$E_f(\mathcal{C}) = I_f(\mu_{\mathcal{C}}), \quad \text{where} \quad \mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x, \tag{1.1.3}$$

and we shall often abuse the terminology by saying that $\mathcal{C}$ (instead of $\mu_{\mathcal{C}}$) minimizes I_f.

In some models, energy minimization leads to a clustering effect, in the sense that the resulting optimal measures tend to be discrete or at least supported on lower dimensional submanifolds. This phenomenon has been repeatedly observed for energies on $\mathbb{R}^d$ with *attractive-repulsive* potentials, which naturally appear in models in computational chemistry, mathematical biology, and social sciences [6, 28, 29, 76, 80, 106, 150, 158].

In the Euclidean setting, one finds often that the above energies are minimized by measures supported on a sphere of some radius. Our results have some implications in this direction, but we concentrate primarily on potentials on the sphere. Those functions $f(\langle x, y \rangle)$ which are increasing near 1, but decreasing near -1; we call *attractive-repulsive* ; meaning two particles x and y experience repulsion when x and y are close, but attract when they are far apart. In some examples, potentials of the energy are also *symmetric* and *orthogonalizing*, i.e. they satisfy $f(t) = f(|t|)$, and $\min\{f(t) : t \in [-1, 1]\} = f(0)$, which results in two particles achieving equilibrium when they are in an orthogonal position.

One of the most interesting energies of this type is the p*-frame energy* corresponding to $f(t) = |t|^p$, where $p > 0$,

$$I_f(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} |\langle x, y \rangle|^p d\mu(x) d\mu(y). \tag{1.1.4}$$

The behavior of minimizing measures of this energy exhibits peculiar phase transitions at even integer values of p. Whenever $p \in 2\mathbb{N}$, the p-frame energy is minimized by the normalized surface measure σ [134, 50], among other measures. However, for $p \notin 2\mathbb{N}$, all the minimizers appear to be discrete. This phenomenon will be a main focus of Chapter 2.

For $p = 2$, this energy and its discrete counterpart, often referred to simply as the *frame potential*, have been studied in [134] and later again in [12]. In the latter paper, which coined the name for this energy, it was proved that the minimizers of the discrete energies with $N \geq d$ points are precisely unit norm *tight frames*. A tight frame is a set of vectors $\{\varphi_i\}_{i=1}^N \subset \mathbb{R}^d$ such that a Parseval type identity,

$$\sum_{i=1}^{N} |\langle x, \varphi_i \rangle|^2 = C\|x\|^2, \tag{1.1.5}$$

holds for all $x \in \mathbb{R}^d$ and for some constant $C > 0$. In other words, tight frames act as overcomplete orthonormal bases and thus play an important role in several areas of applied mathematics. Isotropic measures on the sphere also minimize the continuous frame energy over all probability measures (see equation 2.1.1).

In the case $p = 4$, the p-frame energy is closely connected to the maximal equiangular tight frames, which in the complex case are known as *symmetric informationally complete positive operator-valued measures* (SIC-POVMs). These are unit norm tight frames $\{\varphi_i\}_{i=1}^N$ with the property that $|\langle \varphi_i, \varphi_j \rangle|^2 = \frac{1}{d+2}$ or $\frac{1}{d+1}$ for $i \neq j$, in the real and complex case respectively. In $\mathbb{C}^d$, Zauner's conjecture [162] states that SIC-POVMs exist in all dimensions $d \geq 2$, which is supported by extensive numerical evidence [130, 119]. In the real case, the existence of analogous objects is also mysterious: they may exist only in dimensions $d = 1, 2, 3$, or $d = (2m-1)^2 - 2$ [89], but do not exist for $d = 47$ [98]. When these objects do exist, they minimize the 4-frame energy (with the complex unit sphere replacing $\mathbb{S}^{d-1}$ in the case of SIC-POVMs).

More generally, when $p = 2k \in 2\mathbb{N}$, the function $f(t) = |t|^p = t^{2k}$ is a polynomial, hence any *spherical* $2k$*-design* yields the same value of the p-frame energy as σ, and thus is also a minimizer. More precisely, discrete equal-weight minimizers are exactly *projective* k*-designs*. A spherical t-design is a set $\{x_i\}_{i=1}^N \subset \mathbb{S}^{d-1}$ such that

$$\frac{1}{N}\sum_{i=1}^{N} p(x_i) = \int_{\mathbb{S}^{d-1}} p(x)\, d\sigma(x)$$

holds for any polynomial p on $\mathbb{R}^d$ of degree up to t; see e.g. [44], while a projective k-design is a configuration such that the above identity holds for all polynomials of degree up to $2k$, which contain only even-degree terms. We will discuss spherical and projective designs further in Chapter 2, but to summarize, the p-frame energy has a multitude of minimizers, both continuous and discrete, when p is an even integer.

When $p \notin 2\mathbb{N}$, the situation is much less studied. In Chapter 2, we show that, when certain highly symmetrical configurations exist, they minimize the p-frame energy on a range of values of p between two consecutive even integers. These configurations, known as *tight designs*, (see Definition 2.2.5) are designs of high order with few distinct pairwise distances, or equivalently, designs of smallest possible cardinality [44]. Theorem 2.1.1 in this thesis states that a tight spherical $(2k+1)$-design, whenever it exists, minimizes the p-frame energy for $p \in [2k-2, 2k]$, and, moreover, *every* minimizer for $p \in (2k-2, 2k)$ has to be a tight design (in particular, it has to be discrete). We have accumulated a great deal of numerical evidence that suggests discreteness of minimizers generally (collected in table 2.1), leading us to the following conjecture:

Conjecture 1.1.1. Let $p > 0$ and $p \notin 2\mathbb{N}$. Then every minimizer of the p-frame energy (1.1.4) is a finite discrete measure on $\mathbb{S}^{d-1}$.

There are other conjectures in the literature also asserting the discreteness of measures minimizing certain energies on the sphere. We mention a couple of examples.

Let $f(t) = \arccos|t|$, i.e. $f(\langle x, y\rangle)$ represents the non-obtuse angle between the lines generated by the vectors x and y. A conjecture of Fejes Tóth [51] states that the N-point energy (1.1.1) (the sum of acute angles) is *maximized* by the periodically repeated elements of the orthonormal basis, and the continuous version of the conjecture speculates that I_f is *maximized* by the discrete measure uniformly distributed over the elements of the orthonormal basis (see [14] for more details and recent results).

Another similar conjecture stems from mathematical physics and relativistic quantum field theory [53, 3]. It concerns the *causal variational principle*, which, in the spherical case, concerns minimizing the energy on $\mathbb{S}^2$ with the kernel

$$f(\langle x, y\rangle) = \max\{0,\, 2\tau^2(1 + \langle x, y\rangle)(2 - \tau^2(1 - \langle x, y\rangle))\}, \tag{1.1.6}$$

with a real parameter $\tau > 0$. It is conjectured in [53] that for any $\tau \geq 1$ *there exists* a discrete minimizer, and for $\tau > \sqrt{2}$ *all minimizers* are discrete. In Section A.1.3 it is demonstrated that for two values of τ, minimizers are the cross-polytope and the icosahedron, respectively.

In the present chapter we prove a series of results which establish discreteness of minimizers or smallness of their support (or at least the existence of such minimizers) for various classes of energies on $\mathbb{S}^{d-1}$. In particular, in Theorem 1.3.3 we prove a quantitative version of the following statement:

Theorem 1.1.2. Assume that $f \in C[-1,1]$ has only finitely many positive coefficients in its orthogonal expansion with respect to Gegenbauer polynomials C_n. Then there exists a discrete minimizer of the energy I_f on $\mathbb{S}^{d-1}$.

The cardinality of the support of this discrete minimizer is bounded by the dimension of the space of spherical harmonics, corresponding to the positive coefficients of f. The proof relies on the analysis of the structure of extreme points of the set of moment-constrained measures. Section 1.3 contains a self-contained exposition of these arguments.

While the discreteness of the minimizers claimed in Conjecture 1.1.1 remains out of reach, we establish that the support of the measures minimizing the $p-$frame energy with $p \notin 2\mathbb{N}$ must be small:

Theorem 1.1.3. Assume that $p > 0$ and $p \notin 2\mathbb{N}$, and set $f(t) = |t|^p$. Let $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$ be a minimizer of the p-frame energy I_f (1.1.4). Then the support of μ has empty interior, i.e.

$$(\operatorname{supp}\mu)^\circ = \emptyset.$$

Section 1.4 is devoted to the proof of this theorem. In order to compare this theorem to some known results on $\mathbb{R}^d$, we point out that discreteness of minimizers for attractive-repulsive potentials on $\mathbb{R}^d$ has been proved in [28] under the assumption that f is *mildly repulive*, i.e. that the potential, as a function of $r = |x-y|$, behaves as $-r^\alpha$ for small r, with $\alpha > 2$ (a similar result for spheres appears in [149]). Since on the sphere $|\langle x, y\rangle|^p \approx 1 - \frac{p}{2}r^2$, the p-frame potential corresponds to the endpoint case $\alpha = 2$ and thus is quite delicate: indeed, we know for some values of p there exist non-discrete minimizers. In the recent paper [93] it was shown that for some specific attractive-repulsive potentials with $\alpha \geq 2$, the corresponding energies are uniquely minimized by discrete measures on regular simplices. The complete understanding of the endpoint case $\alpha = 2$ remains an interesting open problem.

In Section 1.5, we also prove that an analog of Theorem 1.1.3 holds for energies with kernels $f : [-1, 1] \to \mathbb{R}$, which are real-analytic, but not positive definite on $\mathbb{S}^{d-1}$ up to an additive constant (see Definition 1.2.1 and Proposition 1.2.2). Theorem 1.5.1 states that for such kernels, minimizing measures have support with empty interior. Moreover, on the circle $\mathbb{S}^1$, they are discrete. This generates a certain dichotomy: for an analytic functions f, either the energy I_f is minimized by the uniform surface measure σ, or *all minimizers* have support with empty interior.

This result, as well as Theorem 1.1.2, obviously applies to polynomials. Thus, when a polynomial f is not positive definite (up to an additive constant), the support of *every* minimizer has empty interior, while for *every* polynomial f there exists a discrete minimizer of I_f (see Corollary 1.6.1). For positive definite polynomials f, discrete minimizers are just *weighted spherical designs*, but for arbitrary polynomials, existence of discrete minimizers is new. Section 1.6 presents a discussion of energies with polynomial kernels.

Finally, in Section 1.7 we present an interesting observation that for positive definite kernels f, any local minimizer of the energy I_f is necessarily a global minimizer. This applies, in particular, to the p-frame energy with even integer values of p and to many other interesting energies.

1.2 Background

1.2.1 Spherical harmonics and Gegenbauer polynomials

For a parameter $\lambda > 0$, consider the weight $\nu(t) = (1 - t^2)^{\lambda - \frac{1}{2}}$ on the interval $[-1, 1]$, where from now on $\lambda = \frac{d-2}{2}$. The weight $\nu(t)$ is related to integration on the sphere $\mathbb{S}^{d-1}$ in the following way: for a unit vector $p \in \mathbb{S}^{d-1}$,

$$\int_{\mathbb{S}^{d-1}} f(\langle x, p \rangle) d\sigma(x) = I_f(\sigma) = \frac{\omega_{d-2}}{\omega_{d-1}} \int_{-1}^{1} f(t)(1 - t^2)^{\frac{d-3}{2}} \, dt, \tag{1.2.1}$$

where, as before, σ is the normalized surface measure on the sphere $\mathbb{S}^{d-1}$ and $\omega_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the $(d-1)$-dimensional Hausdorff surface measure of $\mathbb{S}^{d-1}$.

Gegenbauer polynomials C_n^λ, $n \geq 0$, form a sequence of orthogonal polynomials with respect to the weight $\nu(t)$ on the interval $[-1, 1]$. Every function $f \in L^1([-1,1], \nu(t)dt)$ has a Gegenbauer (ultraspherical) expansion

$$f(t) \sim \sum_{n=0}^{\infty} \widehat{f}_n \frac{n+\lambda}{\lambda} C_n^\lambda(t). \tag{1.2.2}$$

For $f \in L^2([-1,1], \nu(t)dt)$ this expansion converges to f in the L^2 sense. In the case of $\mathbb{S}^1$, when $\lambda = 0$, the relevant polynomials are the Chebyshev polynomials of the first kind

$$T_n(t) = \cos(n \arccos t) = \frac{1}{2} \lim_{\lambda \to 0} \frac{n+\lambda}{\lambda} C_n^\lambda(t), \tag{1.2.3}$$

and for $\mathbb{S}^2$, the polynomials are appropriately scaled Legendre polynomials [141].

Let $\mathcal{H}_n^d$ denote the space of spherical harmonics of order n, the functions which are restrictions to $\mathbb{S}^{d-1}$ of homogeneous harmonic polynomials of degree n on $\mathbb{R}^d$. These spaces are mutually orthogonal for different values of n and satisfy

$$L^2(\mathbb{S}^{d-1}, d\sigma) = \bigoplus_{n=0}^{\infty} \mathcal{H}_n^d.$$

Let $\{Y_{n,j}\}$ be any orthonormal basis in $\mathcal{H}_n^d$. The Gegenbauer polynomials are related to the spherical harmonics by the following *addition formula*

$$\sum_{j=1}^{a_n^d} Y_{n,j}(x) Y_{n,j}(y) = \frac{n+\lambda}{\lambda} C_n^\lambda(\langle x, y \rangle) \quad \text{for all} \quad x, y \in \mathbb{S}^{d-1}, \tag{1.2.4}$$

where

$$a_n^d = \dim \mathcal{H}_n^d = \frac{n+\lambda}{\lambda} C_n^\lambda(1) = \frac{2n+d-2}{n+d-2} \binom{n+d-2}{d-2}.$$

For more detailed information on spherical harmonics, Gegenbauer polynomials, and harmonic analysis on the sphere, we refer the reader to [40, 109].

1.2.2 Positive definite functions on $\mathbb{S}^{d-1}$.

Positive definite functions play an important role in energy minimization.

Definition 1.2.1. A function $f \in C[-1,1]$ is positive definite on subset K of sphere $\mathbb{S}^{d-1}$, if for every collection of points $\{x_i\}_{i=1}^N \subset K$, the matrix $[f(\langle z_i, z_j\rangle)]_{i,j=1}^N$ is positive semidefinite, i.e. for any sequence $\{c_i\}_{i=1}^N \subset \mathbb{C}$, f satisfies the inequality

$$\sum_{i,j=1}^N c_i \bar{c}_j f(\langle x_i, x_j\rangle) \geq 0.$$

When $K = \mathbb{S}^{d-1}$ is the entire sphere, positive definite functions admit several equivalent characterizations, which connect this property to Gegenbauer polynomials and energy.

Proposition 1.2.2. Let $f \in C[-1,1]$. The following statements are equivalent:

(i) The function f is positive definite on $\mathbb{S}^{d-1}$.

(ii) For any signed Borel measure ν on $\mathbb{S}^{d-1}$, $I_f(\nu) \geq 0$.

(iii) The coefficients in the ultraspherical expansion (1.2.2) of f with respect to Gegenbauer polynomials C_n^λ are non-negative: $\widehat{f}_n \geq 0 \;$ for all $\; n \geq 0$.

(iv) The minimum of the energy I_f over Borel probability measures on $\mathbb{S}^{d-1}$ is achieved by σ and is non-negative, i.e.

$$\min_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) = I_f(\sigma) \geq 0.$$

Part (iii) of this proposition is a classical result due to Schoenberg [129]. Part (iv) states that positive definite functions (up to additive constants) are precisely those potentials for which energy minimization imposes uniform distribution. We give a proof of this statement in the next chapter (see Proposition 2.2.3).

Positive definiteness also implies uniform convergence of the Gegenbauer expansion (1.2.2); see e.g. [62].

Lemma 1.2.3. Assume that $f \in C[-1,1]$ is positive definite on $\mathbb{S}^{d-1}$. Then the Gegenbauer expansion (1.2.2) converges to f absolutely and uniformly on $[-1,1]$.

One of the simplest ways to prove this statement is using Mercer's theorem from spectral theory on the representation of symmetric positive definite functions [104]. In turn, Lemma 1.2.3 together with the addition formula (1.2.4) easily imply part (iv) of Proposition 1.2.2.

Positive definiteness also plays a role when the energy is not minimized by the uniform measure σ. In this case, we have the following implication [17, 53].

Lemma 1.2.4. Let $f \in C([-1,1])$. Assume that μ is a minimizer of I_f over $\mathcal{P}(\mathbb{S}^{d-1})$ and $I_f(\mu) \geq 0$. Then the function f must be positive definite on $\operatorname{supp}(\mu)$.

Observe that, together with part (iv) of Proposition 1.2.2, this immediately implies the following:

Corollary 1.2.5. Either σ is a minimizer of I_f (i.e. f is positive definite on $\mathbb{S}^{d-1}$, up to an additive constant), or every minimizer of I_f is supported on a proper subset of the sphere $\mathbb{S}^{d-1}$.

Much of this chapter is dedicated to obtaining various refinements of this principle for various classes of kernels f. Lemma 1.2.4 also suggests an approach to proving that a certain set cannot be contained in the support of a minimizer: one may attempt to prove that f is not positive definite on that set. This idea, albeit not in a straightforward fashion, is exploited in the proof of Theorem 1.1.3 in the next section; see the proof of Proposition 1.4.2.

1.2.3 Gegenbauer expansions and other minimizers

In some situations, Gegenbauer coefficients can give some information about the minimizers, even when σ does not minimize the energy. Below we mention several relevant results of this type. While we do not use them in this chapter, we chose to include them because they are similar in spirit to the results here: they provide certain conditions, under which *there exist* discrete minimizers or *all* minimizers are discrete. These results can be found in [13].

- If $\widehat{f}_n \le 0$ for all $n \ge 1$, then a Dirac delta mass $\mu = \delta_z$, for any $z \in \mathbb{S}^{d-1}$, is a minimizer of I_f. If f has a strict absolute minimum at $t = 1$ (in particular, if $\widehat{f}_n < 0$ for all $n \ge 1$), then every minimizer is a Dirac mass. Observe that this case resonates with Theorem 1.3.3.

- If $(-1)^{n+1}\widehat{f}_n \ge 0$ for all $n \ge 1$, then the measure $\mu = \frac{1}{2}(\delta_z + \delta_{-z})$ is a minimizer of I_f. Moreover, all minimizers are of this form, if the strict inequality $(-1)^{n+1}\widehat{f}_n > 0$ holds.

- If $\widehat{f}_{2n} = 0$ and $\widehat{f}_{2n-1} \ge 0$ for all $n \ge 1$, then every centrally symmetric measure minimizes I_f. In particular, there exist discrete minimizers.

We note that for the Euclidean setting, and certain attractive-repulsive potentials, there are classifications of potentials for which two-point measures appear as minimizers, see [76].

1.3 Existence of discrete minimizers

1.3.1 Extreme points for sets of moment-constrained measures

In the present section we exhibit a large class of potentials f for which there exist discrete minimizers of the energies I_f. The methods that we employ are closely related to *moment problems*.

Let Ω be a compact metric space and let $\mathcal{B}_+(\Omega)$ denote the set of positive Borel measures on Ω. Given continuous functions $f_0, ..., f_n$ on Ω and non-negative constants c_i, we consider the set

$$K = \left\{ \mu \in \mathcal{B}_+(\Omega) : \int_\Omega f_i d\mu = c_i,\ i = 0, 1, \dots, n \right\}, \tag{1.3.1}$$

which consists of Borel measures whose moments with respect to $f_i \in C(\Omega)$ are fixed. We always set $f_0 \equiv 1$ and $c_0 = 1$, so that $\mu \in K$ guarantees that μ is a probability measure, i.e. $\mu(\Omega) = 1$.

It is easy to see that K is convex, bounded, and weak-$*$ closed, and therefore is weak-$*$ compact. By the Krein–Milman theorem, K is the weak-$*$ closure of $\mathrm{ext}(K)$ — the set of extreme points of K. The results presented below describe the structure of $\mathrm{ext}(K)$, in particular, the discreteness of its elements. To make this section self-contained, we include their proofs.

We start with a theorem which gives a necessary condition for μ to be an extreme point of K.

Theorem 1.3.1 (Douglas, [48]). Assume that $\mu \in \operatorname{ext}(K)$. Then

$$L^1(d\mu) = \operatorname{span}\{f_0 = 1, f_1, \dots, f_n\}. \tag{1.3.2}$$

Proof. Assume that $g \in L^\infty(d\mu)$ satisfies

$$\int_\Omega f_i g d\mu = 0, \qquad i = 0, 1, \dots, n.$$

Multiplying g by a constant, we may assume that $\|g\|_{L^\infty(d\mu)} < 1$. Then the measures $\mu_\pm$, defined by $d\mu_\pm = (1 \pm g)d\mu$, belong to K, since $\mu_\pm \in \mathcal{B}_+(\Omega)$ and

$$\int_\Omega f_i d\mu_\pm = \int_\Omega f_i(1 \pm g)d\mu = \int_\Omega f_i d\mu = c_i.$$

At the same time, $\mu = \frac{1}{2}(\mu_- + \mu_+)$. Since $\mu \in \operatorname{ext} K$, this implies that $\mu_\pm = \mu$ and hence $g = 0$ μ-a.e. Therefore, the functions f_i span $L^1(d\mu)$. $\square$

We now state and prove a result, which demonstrates the discreteness of the elements of $\operatorname{ext}(K)$. This result has a number of precursors and extensions, see [121, 122, 123, 124, 156, 165].

Theorem 1.3.2 (Karr, [77]). Let $\mu \in K$. Then the following statements are equivalent:

(i) $\mu \in \operatorname{ext}(K)$.

(ii) The cardinality of $\operatorname{supp}\mu$ is at most $n+1$. Moreover, if we denote $\operatorname{supp}\mu = \{x_1, \dots, x_k\}$, then the vectors $v_j = (1, f_1(x_j), \dots, f_n(x_j))$, $j = 1, 2, \dots, k$, are linearly independent.

Proof. (i)⇒(ii). Assume that there exist points $\{x_1, \dots, x_{n+2}\} \subset \operatorname{supp}\mu$. Then one can find a vector $y \in \mathbb{R}^{n+2}$, which is not in the span of the vectors $(f_i(x_1), f_i(x_2), \dots, f_i(x_{n+2}))$, $i = 0, 1, \dots, n$, since the latter subspace is at most $n+1$ dimensional. Appealing to Urysohn's lemma, one can construct a function $g \in C(\Omega) \subset L^1(d\mu)$ such that $g(x_i) = y_i$ for $i = 1, 2, \dots, n+2$. But then $g \notin \operatorname{span}\{f_i\}$, which contradicts Theorem 1.3.1, i.e. $|\operatorname{supp}\mu| \leq n+1$.

Now that it is known that $\mu = \sum_{i=1}^{k} t_i \delta_{x_i}$ with $k \le n+1$, $t_i > 0$, $\sum t_i = 1$, consider the linear system

$$\begin{pmatrix} 1 & \dots & 1 \\ f_1(x_1) & \dots & f_1(x_k) \\ \vdots & \ddots & \vdots \\ f_n(x_1) & \dots & f_n(x_k) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_k \end{pmatrix} = \begin{pmatrix} 1 \\ c_1 \\ \vdots \\ c_n \end{pmatrix}. \tag{1.3.3}$$

This system has a unique solution $\alpha_i = t_i$, since if the solution is not unique, then there is a whole affine subspace of solutions and one could perturb the values of t_i in opposite directions, i.e. find two solutions of the form $\{t_i \pm \tau_i\}$, and construct two measures $\mu_\pm = \sum_{i=1}^{k} (t_i \pm \tau_i)\delta_{x_i}$ so that $\mu_\pm \ge 0$ and $\int f_i d\mu_\pm = \int f_i d\mu$, i.e. $\mu_\pm \in K$, and $\mu = \frac{1}{2}(\mu_+ + \mu_-)$, which contradicts the fact that $\mu \in \mathrm{ext}(K)$. This proves the linear independence of the rows of the matrix above.

(ii)⇒(i). Assume that (ii) holds. Then the system (1.3.3) has a unique solution, i.e. μ is uniquely determined by the the condition $\operatorname{supp} \mu \subset \{x_1, \dots, x_k\}$. If $\mu = \frac{1}{2}(\mu_1 + \mu_2)$, then $\operatorname{supp} \mu \subset \operatorname{supp} \mu_1 \cup \operatorname{supp} \mu_2$, and thus $\operatorname{supp} \mu_j \subset \{x_1, \dots, x_k\}$ for $j = 1, 2$. Therefore $\mu_1 = \mu_2 = \mu$, i.e. $\mu \in \mathrm{ext}(K)$. $\square$

We remark that convex geometry plays heavily into similar characterizations of solutions to infinite dimensional optimization problems in the recent papers [21, 31, 147].

1.3.2 Applications of Karr's theorem: existence of discrete minimizers.

We now apply the results on moment-constrained measures to prove that for a function f with only finitely many positive terms in its Gegenbauer expansion, there exist discrete minimizers of I_f.

Let $\widehat{f}_n$ denote the coefficients in the Gegenbauer expansion (1.2.2) of the function $f \in C[-1,1]$. Consider the sets $N_+(f) = \{n \ge 0 : \widehat{f}_n > 0\}$ and $N_-(f) = \{n \ge 0 : \widehat{f}_n < 0\}$. We shall assume that

$$|N_+(f)| < \infty, \tag{1.3.4}$$

i.e. there are only finitely many terms of (1.2.2) with $\widehat{f}_n > 0$. In this case, the function

$$\sum_{n \in N_+(f)} \widehat{f}_n \frac{n+\lambda}{\lambda} C_n^\lambda(t) - f(t)$$

is continuous and positive definite. According to Lemma 1.2.3, this implies that the Gegenbauer expansion (1.2.2) of f converges uniformly and absolutely.

Recall that $\mathcal{H}_n^d$ denotes the space of spherical harmonics of degree n on $\mathbb{S}^{d-1}$. We are now ready to state the main theorem of the section.

Theorem 1.3.3. Assume that the Gegenbauer expansion (1.2.2) of the function $f \in C[-1,1]$ satisfies

$$|N_+(f)| = |\{n \geq 0 : \widehat{f}_n > 0\}| < \infty,$$

i.e. the Gegenbauer expansion has only finitely many positive terms. Then there exists a discrete measure $\mu^* \in \mathcal{P}(\mathbb{S}^{d-1})$ such that

$$|\operatorname{supp} \mu^*| \leq \sum_{n \in N_+(f) \cup \{0\}} \dim \mathcal{H}_n^d, \tag{1.3.5}$$

and μ^* minimizes the energy $I_f(\mu)$ over $\mathcal{P}(\mathbb{S}^{d-1})$, i.e.

$$I_f(\mu^*) = \inf_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu). \tag{1.3.6}$$

Proof. Let $\nu \in \mathcal{P}(\mathbb{S}^{d-1})$ be any minimizer of I_f and set

$$M = \inf_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) = I_f(\nu).$$

We shall use the addition formula for spherical harmonics (1.2.4), as well as the absolute convergence of (1.2.2), to re-write for any measure $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$, $I_f(\mu)$ as,

$$\sum_{n=0}^{\infty} \widehat{f}_n \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \frac{n+\lambda}{\lambda} C_n^{\lambda}(\langle x, y\rangle) d\mu(x) d\mu(y) = \sum_{n=0}^{\infty} \widehat{f}_n \left[\sum_{j=1}^{\dim \mathcal{H}_n^d} \left(\int_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right]$$

$$= \sum_{n \in N_+(f)} \widehat{f}_n \left[\sum_{j=1}^{\dim \mathcal{H}_n^d} \left(\int_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right] - \sum_{n \in N_-(f)} (-\widehat{f}_n) \left[\sum_{j=1}^{\dim \mathcal{H}_n^d} \left(\int_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right],$$

the last of which we define as the difference of functionals $\mathcal{F}(\mu) - \mathcal{G}(\mu)$. It is easy to see that $\mathcal{G}$ is convex with respect to μ since it is a positive linear combination of squares of linear functionals of μ. Let us set

$$K = \left\{ \mu \in \mathcal{B}_+(\mathbb{S}^{d-1}) : \int_{\mathbb{S}^{d-1}} Y_{n,j} d\mu(x) = \int_{\mathbb{S}^{d-1}} Y_{n,j} d\nu(x),\, n \in N_+(f),\, j = 1, 2, \ldots, \dim \mathcal{H}_n^d \right\},$$

so that $\nu \in K$ and $\mathcal{F}(\mu) = \mathcal{F}(\nu)$ for $\mu \in K$. Without loss of generality, we shall assume that $0 \in N_+(f)$. This guarantees that $\mu \in K$ is a probability measure (similarly to setting $c_0 = 1$ and $f_0 \equiv 1$ earlier). Since $N_+(f) < \infty$, the set K has finitely many moment constraints and Theorem 1.3.2 is applicable. In fact, the number of constraints is exactly the right-hand side of (1.3.5).

Given that $\mathcal{G}$ is convex in μ and K is a convex weak-$*$ compact subset of $\mathcal{B}_+(\mathbb{S}^{d-1})$, we conclude that $\mathcal{G}(\mu)$ achieves its maximum on K at a point of $\mathrm{ext}(K)$. Hence there exists a measure $\mu^* \in \mathrm{ext}(K)$ such that $\mathcal{G}(\mu^*) = \sup\limits_{\mu \in K} \mathcal{G}(\mu)$. We then find that

$$\begin{aligned} M = \inf_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) &= I_f(\nu) = \mathcal{F}(\nu) - \mathcal{G}(\nu) = \mathcal{F}(\mu^*) - \mathcal{G}(\nu) \\ &\geq \mathcal{F}(\mu^*) - \mathcal{G}(\mu^*) = I_f(\mu^*) \geq M, \end{aligned}$$

i.e. $I_f(\mu^*) = M$ and μ^* is also a minimizer of I_f.

Since $\mu^* \in \mathrm{ext}(K)$, we can apply Karr's theorem (Theorem 1.3.2) to finish the proof of the theorem. $\square$

1.4 Empty interior of p-frame energy minimizers: the proof of Theorem 1.1.3

Conjecture 1.1.1, stating that the minimizers of the p-frame energy with $p \notin 2\mathbb{N}$ are necessarily discrete, remains open, outside of some specific cases covered in Chapter 2. In the present section, we prove a weaker statement, namely, that the support of every minimizer of such energies has empty interior, i.e. Theorem 1.1.3.

A similar result has been proved in [53] for the energy on $\mathbb{S}^2$ with the kernel given by (2.8.4). While our approach is inspired by theirs and the main line of reasoning follows an analogous path, specific constructions and arguments in the proofs of Propositions 1.4.2 and 1.4.3 below are much more peculiar and significantly more involved in the case of the p-frame energy.

We shall need a standard fact from potential theory ([17, 19, 86]). For a measure $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$, let us define the *potential* F_μ of μ with respect to f as

$$F_\mu(x) := \int_{\mathbb{S}^{d-1}} f(\langle x, y \rangle) d\mu(y), \quad x \in \mathbb{S}^{d-1}. \tag{1.4.1}$$

Notice that this meaning of the term "potential" is consistent with our previous usage, since the function $f(\langle x, y \rangle)$ is just the potential generated by a unit point charge at y, i.e. $f(\langle x, y \rangle) = F_{\delta_y}(x)$. It is a well-known phenomenon from electrostatics that the potential of the equilibrium measure is constant on the support of the measure.

Lemma 1.4.1. If $f \in C([-1, 1])$ and μ is a minimizer of I_f, then the potential F_μ is constant on the support of μ:

$$F_\mu|_{\operatorname{supp} \mu} = \inf_{x \in \mathbb{S}^{d-1}} F_\mu(x) = I_f(\mu). \tag{1.4.2}$$

In what follows, the value of $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$ is fixed, $f(t) = |t|^p$, and μ is assumed to be a minimizer of I_f. The proof of Theorem 1.1.3 is based on two properties of interior points of $\operatorname{supp}(\mu)$.

Proposition 1.4.2. Let $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$, $f(t) = |t|^p$, and μ be a minimizer of I_f. Then for $z \in$

$(\operatorname{supp}\mu)^\circ$,

$$\operatorname{supp}\mu \cap z^\perp = \emptyset.$$

Proposition 1.4.3. Let the same conditions as in Proposition 1.4.2 hold. Then for $z \in (\operatorname{supp}\mu)^\circ$,

$$\operatorname{supp}\mu \cap z^\perp \neq \emptyset.$$

Since these two statements are clearly mutually exclusive whenever $\operatorname{supp}\mu$ is non-empty, their validity proves Theorem 1.1.3, i.e. that there are no interior points in the support of a minimizer. The remainder of this section is dedicated to the proof of these propositions.

We now sketch the argument for the first proposition. In short, the idea of the proof is the following. Assume that there exists a point $y \in \operatorname{supp}\mu$ such that $\langle y, z\rangle = 0$. We shall construct a finite set of points $X = \{x_i\}_{i=1}^N \subset \operatorname{supp}\mu$, such that the matrix $[f(\langle x_i, x_j\rangle)]_{i,j}$ is not positive semidefinite, thus violating Lemma 1.2.4. The set X will consist of the points z, y, and a number (depending on p) of points, equidistantly spaced around z on the great circle connecting y and z. We now make this precise.

The proof of Proposition 1.4.2. We prove that if z is an interior point of a minimizer's support, then the orthogonal hyperplane $z^\perp$ does not intersect the support of μ.

Fix z in the interior of $\operatorname{supp}(\mu)$ and let $y \in \mathbb{S}^{d-1}$ be any point such that $\langle y, z\rangle = 0$. Setting $k \in \mathbb{N}$ so that $2k-2 < p < 2k$, we shall construct a set $\{x_0, \dots, x_{N-1}\}$ of $N = 2k+2$ points, all of which lie on the great circle connecting z and y. The points $x_0, \dots, x_{2k}$ are chosen in such a way that the angle between x_j and z is $(j-k)\varepsilon$ for some small $\varepsilon > 0$. Thus $x_k = z$, and the points x_0 and x_{2k} make angles $-k\varepsilon$ and $k\varepsilon$ with z, respectively. Observe that when ε is small enough, all of these points $x_0, \dots, x_{2k}$ belong to $\operatorname{supp}(\mu)$, since z is an interior point. Finally, we set $x_{2k+1} = y$. Then the angle between $x_{2k+1} = y$ and x_j, $j = 0, \dots, 2k$, is $\frac{\pi}{2} - (j-k)\varepsilon$. In order to apply Lemma 1.2.4, we consider the matrix $A = [f(\langle x_i, x_j\rangle)]_{i,j=0}^{2k+1}$.

We will show that the matrix A is not positive semidefinite. To this end, we first construct an auxiliary vector $v \in \mathbb{R}^{2k+1} \setminus \{0\}$ such that for $m \in \{0, 1, ..., 2k-1\}$,

$$\sum_{j=0}^{2k} j^m v_j = 0, \tag{1.4.3}$$

i.e. this vector must be in the (right) kernel of the Vandermonde matrix

$$\begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 2 & 3 & \cdots & 2k \\ 0 & 1 & 2^2 & 3^2 & \cdots & (2k)^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2^{2k-1} & 3^{2k-1} & \cdots & (2k)^{2k-1} \end{pmatrix}.$$

We can take the entries of v to be

$$v_j = \prod_{\substack{i=0 \\ i \neq j}}^{2k} \frac{1}{j-i} = \frac{(-1)^j}{(2k-j)!\, j!}. \tag{1.4.4}$$

Such a vector can be seen to be in the kernel of the matrix above by use of the formula for the inverse of the square Vandermonde matrix (see Ex. 40 on page 38 of [78]).

Consider a vector $u = [\alpha v_0, \alpha v_1, ..., \alpha v_{2k}, \beta]^T \in \mathbb{R}^{2k+2}$, where α, $\beta \in \mathbb{R}$. Then we have

$$\langle Au, u \rangle = \alpha^2 \left(\sum_{i,j=0}^{2k} v_i v_j f(\langle x_i, x_j \rangle) \right) + 2\alpha\beta \left(\sum_{j=0}^{2k} v_j f(\langle x_{2k+1}, x_j \rangle) \right) + \beta^2. \tag{1.4.5}$$

We shall show that the real numbers α and β can be chosen in such a way that the expression above is negative, for ε sufficiently small.

Observe that for i, $j = 0, \ldots, 2k$ we have

$$f(\langle x_i, x_j \rangle) = \cos^p((i-j)\varepsilon).$$

Since $\cos^p(t)$ is even, smooth near zero, and $\cos^p(0) = 1$, we can use its Taylor expansion to estimate the first term of (1.4.5) as follows

$$\begin{aligned}\sum_{i,j=0}^{2k} v_i v_j f(\langle x_i, x_j\rangle) &= \sum_{i,j=0}^{2k} v_i v_j \cos^p((i-j)\varepsilon) \\ &= \sum_{i,j=0}^{2k} v_i v_j \left(1 + \sum_{m=1}^{2k-1} a_m \varepsilon^{2m}(i-j)^{2m} + O(\varepsilon^{4k})\right) \\ &= \left(\sum_{j=0}^{2k} v_j\right)\left(\sum_{i=0}^{2k} v_i\right) + \sum_{m=1}^{2k-1} a_m \varepsilon^{2m}\left(\sum_{i,j=0}^{2k} v_i v_j (i-j)^{2m}\right) + O(\varepsilon^{4k}) \\ &= \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} \sum_{i,j=0}^{2k} v_i v_j \sum_{l=0}^{2m} \binom{2m}{l} i^l j^{2m-l} + O(\varepsilon^{4k}) \\ &= \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} \sum_{l=0}^{2m} \binom{2m}{l}\left(\sum_{i=0}^{2k} v_i i^l\right)\left(\sum_{j=0}^{2k} v_j j^{2m-l}\right) + O(\varepsilon^{4k}) \\ &= O(\varepsilon^{4k}),\end{aligned} \tag{1.4.6}$$

where we have used the fact that for all values of $l = 0, 1, \ldots, 2m$, either $l \leq 2k-1$ or $2m - l \leq 2k - 1$.

We now turn to the second term of (1.4.5). Observe that for $j = 0, \ldots, 2k$ we have

$$f(\langle x_{2k+1}, x_j\rangle) = f(\langle y, x_j\rangle) = \cos^p\left(\frac{\pi}{2} - (j-k)\varepsilon\right) = |\sin((j-k)\varepsilon)|^p. \tag{1.4.7}$$

We then find that

$$\begin{aligned}\sum_{j=0}^{2k} v_j f(\langle y, x_j\rangle) &= \sum_{j=0}^{2k} v_j \sin^p(|k-j|\varepsilon) = \sum_{j=0}^{2k} v_j \left(|k-j|\varepsilon + O(\varepsilon^3)\right)^p \\ &= \sum_{j=0}^{2k} v_j (|k-j|\varepsilon)^p \left(1 + O(\varepsilon^2)\right)^p = \varepsilon^p \sum_{j=0}^{2k} v_j |k-j|^p + O(\varepsilon^{p+2}).\end{aligned} \tag{1.4.8}$$

We now analyze the coefficient of ε^p in the above expression using (1.4.4)

$$\sum_{j=0}^{2k} v_j |k-j|^p = \sum_{j=0}^{2k} (-1)^j \frac{|k-j|^p}{(2k-j)!\, j!} = 2\sum_{j=0}^{k-1} (-1)^j \frac{(k-j)^p}{(2k-j)!\, j!}.$$

Since the above is a sum of k exponential functions of p, we know that $\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!}$ has at most $k-1$ zeros, see e.g. Ex. 75 from [115, pg. 46]. We will show that these zeros are exhausted by the even integer values $p = 2, 4, \ldots, 2k-2$. Indeed, assume indirectly that

$$2\sum_{j=0}^{k-1} (-1)^j \frac{(k-j)^p}{(2k-j)!\, j!} = b \neq 0$$

for some even integer $0 < p \leq 2k-2$. Then according to (1.4.5), (1.4.6), and (1.4.8) we have

$$\langle Au, u\rangle = \alpha^2 O(\varepsilon^{4k}) + 2\alpha\beta \left(b\varepsilon^p + O(\varepsilon^{p+2})\right) + \beta^2.$$

Since $p < 2k$, for ε sufficiently small, the discriminant of this quadratic form is positive, hence we can choose α and β so that $\langle Au, u\rangle < 0$. However, since $f(t) = |t|^p$ is a positive definite function on $\mathbb{S}^{d-1}$ for even integer p, this is a contradiction, as the matrix A must be positive semidefinite for any collection $\{x_i\}$. Therefore

$$2\sum_{j=0}^{k-1} (-1)^j \frac{(k-j)^p}{(2k-j)!\, j!} = 0$$

for all $p \in \{2, 4, ..., 2k-2\}$. Since there are at most $k-1$ zeros of this function, we then know that

$$b_p := 2\sum_{j=0}^{k-1} (-1)^j \frac{(k-j)^p}{(2k-j)!\, j!} \neq 0$$

for all other values of p. Let $p \in (0, 2k) \setminus \{2, 4, ..., 2k-2\}$. Then

$$\langle Au, u\rangle = \alpha^2 O(\varepsilon^{4k}) + 2\alpha\beta \left(b_p\varepsilon^p + O(\varepsilon^{p+2})\right) + \beta^2,$$

and by the previous argument, for ε sufficiently small, we could choose α and β so that $\langle Au, u\rangle < 0$, i.e. A is not positive definite. Thus, according to Lemma 1.2.4, $\{x_0, x_1, ..., x_{2k}, y\}$ is not a subset of $\operatorname{supp}\mu$. Since, by assumption, for small $\varepsilon > 0$ the points $x_0, x_1, \ldots, x_{2k}$ all lie in a neighborhood of z and hence in $\operatorname{supp}\mu$, this implies that $y \notin \operatorname{supp}\mu$ and so $\operatorname{supp}\mu \cap z^\perp = \emptyset$. $\square$

We would like to make the following remark. Observe that for $p \notin 2\mathbb{N}$, the number of points used to disprove positive definiteness of $f(t) = |t|^p$ in the argument above is of the order p. A restriction of this type is actually necessary. Indeed, according to the result of Fitzgerald and Horn [54], for any positive definite matrix $A = [a_{ij}]_{i,j=1}^N$ with non-negative entries $a_{ij} \geq 0$, its Hadamard powers $A^{(\alpha)} = [a_{ij}^\alpha]_{i,j=1}^N$ are also positive definite when $\alpha \geq N - 2$. Let $G = [\langle x_i, x_j\rangle]_{i,j=1}^N$ be the Gram matrix of the set $X = \{x_1, \ldots, x_N\} \subset \mathbb{S}^{d-1}$. Since the matrix $G^{(2)} = [|\langle x_i, x_j\rangle|^2]_{i,j=1}^N$ is positive definite and has non-negative entries, we have that the matrix

$$G^{(p)} = [|\langle x_i, x_j\rangle|^p]_{i,j=1}^N = (G^{(2)})^{(p/2)}$$

is positive definite whenever $p/2 \geq N - 2$. Therefore, to obtain a non-positive definite matrix $G^{(p)}$, we must take $N \geq 2 + p/2$ points.

We now complete the proof of Theorem 1.1.3.

The proof of Proposition 1.4.3. Suppose a neighborhood of a point $z \in \mathbb{S}^{d-1}$ is contained in the support of μ. We shall demonstrate that $\operatorname{supp}\mu$ must intersect the hyperplane $z^\perp$.

Let us assume the contrary, i.e. $\operatorname{supp}\mu \cap z^\perp = \emptyset$. We may move all the mass of μ to the hemisphere centered at z by defining a new measure $\mu_z \in \mathcal{P}(\mathbb{S}^{d-1})$:

$$\mu_z(E) = \begin{cases} \mu(-E \cup E), & \text{if } E \subseteq \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle > 0\}, \\ \mu(E), & \text{if } E \subseteq z^\perp, \\ 0, & \text{if } E \subseteq \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle < 0\}. \end{cases}$$

Since $f(\langle z, y\rangle) = f(\langle z, -y\rangle)$ for all $y \in \mathbb{S}^{d-1}$, this does not change the energy, i.e. $I_f(\mu_z) = I_f(\mu)$, so that μ_z is also a minimizer.

Since $\operatorname{supp}\mu \cap z^\perp = \emptyset$, we also have that $\operatorname{supp}\mu_z \cap z^\perp = \emptyset$, i.e. $\operatorname{supp}\mu_z \subset \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle > 0\}$. Compactness of the support of μ_z then implies that it is separated from $z^\perp$, i.e. for some $\delta > 0$ we have $\langle y, z\rangle > \delta$ for each $y \in \operatorname{supp}\mu_z$. Let us choose an open neighborhood U_z of z, small enough so that $U_z \subset \operatorname{supp}\mu_z$ and so that for each $x \in U_z$ and each $y \in \operatorname{supp}\mu_z$, $\langle y, x\rangle > \delta > 0$.

We can now write the potential (1.4.1) of μ_z at the point $x \in U_z$ as

$$F_{\mu_z}(x) = \int_{\mathbb{S}^{d-1}} |\langle x, y\rangle|^p \, d\mu_z(y) = \int_{\operatorname{supp}\mu_z} \langle x, y\rangle^p \, d\mu_z(y). \tag{1.4.9}$$

The discussion above implies that the last expression is well-defined for all $p > 0$. According to Lemma 1.4.1, the potential $F_{\mu_z}(x)$ is constant on $U_z \subset \operatorname{supp}\mu_z$.

When p is an odd integer, the proof can be finished very quickly. Indeed, in this case the expression

$$g(x) = \int_{\operatorname{supp}\mu_z} \langle x, y\rangle^p \, d\mu_z(y)$$

is well defined for each $x \in \mathbb{S}^{d-1}$ and yields an analytic function on the sphere (actually, a polynomial). Hence, being constant on an open set, implies that it is is constant on all of $\mathbb{S}^{d-1}$, which is not possible since, obviously, $g(-z) = -g(z) = -F_{\mu_z}(z) = -I_f(\mu_z) \neq 0$. Compare this argument to Theorem 1.5.1.

We now will present an approach which works for all $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$. Assume that there exists a differential operator D acting on functions on the sphere with the following two properties:

(i) D locally annihilates constants, i.e. if $u(x)$ is constant on some open set Ω, then $D_x u = 0$ on Ω;

(ii) $D_x\left(\langle x, y\rangle^p\right) < 0$ for all $x \in U_z$ and $y \in \operatorname{supp}\mu_z$.

Existence of such an operator would finish the proof since we would then have for each $x \in U_z$

$$0 = D_x F_{\mu_z}(x) = \int_{\mathrm{supp}(\mu_z)} D_x\left(\langle x, y\rangle^p\right)\, d\mu_z(y) < 0, \tag{1.4.10}$$

which is a contradiction. Note that switching to $D_x\left(\langle x, y\rangle^p\right) > 0$ in condition (ii) does not affect the proof.

We now construct such an operator D. Let Δ denote the Laplace–Beltrami operator on $\mathbb{S}^{d-1}$. Writing it in the standard spherical coordinates $\vartheta_1, \ldots, \vartheta_d$ one obtains (see, e.g., equation (2.2.4) in [84])

$$\Delta = \sum_{j=1}^{d-1} \frac{1}{q_j (\sin\vartheta_j)^{d-1-j}} \frac{\partial}{\partial \vartheta_j}\left((\sin\vartheta_j)^{d-1-j} \frac{\partial}{\partial\vartheta_j}\right), \tag{1.4.11}$$

where $q_1 = 1$ and $q_j = (\sin\vartheta_1 \ldots \sin\vartheta_{j-1})^2$ for $j > 1$.

For a fixed $y \in \mathbb{S}^{d-1}$, choose the coordinates so that $\cos\vartheta_1 = \langle y, x\rangle$. Then $\langle y, x\rangle^p = \cos^p \vartheta_1$, effectively leaving just one term in the formula above, and a direct computation shows that

$$\Delta_x\left(\langle x, y\rangle^p\right) = p(p-1)\langle x, y\rangle^{p-2} - p(p+d-1)\langle x, y\rangle^p. \tag{1.4.12}$$

Observe that if $p \in (0, 1]$, then the operator Δ_x satisfies conditions (i) and (ii), hence completing the proof for this range of p.

Now consider the operator $D = \Delta\left(\Delta + p(p+d-1)\right)$. It is easy to see that

$$\begin{aligned}\Delta_x\left(\Delta_x + p(p+d-1)\right)\left(\langle x, y\rangle^p\right) &= p(p-1)\Delta_x\left(\langle x, y\rangle^{p-2}\right) \\ &= p(p-1)(p-2)\langle x, y\rangle^{p-4} \cdot \left((p-3) - (p+d-3)\langle x, y\rangle^2\right).\end{aligned} \tag{1.4.13}$$

If $p \in (2, 3]$, then $p - 3 \leq 0$ and $p + d - 3 > d - 1 \geq 0$, so the expression above is strictly negative. Hence this operator satisfies conditions (i) and (ii) for $2 < p \leq 3$.

Moreover, if $p \in (1, 2)$, the expression above is strictly positive. Indeed, the function

$g_p(t) = (p-3) - (p+d-3)t$ is monotone on $[0,1]$ with $g_p(0) = p-3 < 0$ and $g_p(1) = -d < 0$. Therefore, condition (ii) holds with an opposite inequality sign, so the case $1 < p < 2$ is also covered.

It is now clear how to iterate this process. Define now the operator $D^{(0)} = \Delta$, $D^{(1)} = \Delta\,(\Delta + p(p+d-1))$, and, more generally, for $k \in \mathbb{N}$, define the differential operator of order $2k+2$

$$D^{(k)} = \Delta \left(\Delta + (p+d-2k+1) \prod_{j=0}^{2k-2} (p-j) \right) \cdots \left(\Delta + p(p-1)(p-2)(p+d-3) \right) (\Delta + p(p+d-1)). \tag{1.4.14}$$

Let $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$ and choose $k \in \mathbb{N}_0$ so that $2k-1 < p \leq 2k+1$. An iterative computation shows that

$$\begin{aligned} D_x^{(k)} \left(\langle x,y \rangle^p \right) &= \left(\prod_{j=0}^{2k+1} (p-j) \right) \langle x,y \rangle^{p-2k-2} - \left(\prod_{j=0}^{2k} (p-j) \right) (p+d-2k-1) \langle x,y \rangle^{p-2k} \\ &= \left(\prod_{j=0}^{2k} (p-j) \right) \langle x,y \rangle^{p-2k-2} \cdot \left((p-2k-1) - (p+d-2k-1) \langle x,y \rangle^2 \right). \end{aligned} \tag{1.4.15}$$

For $p \in (2k, 2k+1]$, the expression above is strictly negative, since $p - 2k - 1 \leq 0$ and $p + d - 2k - 1 > d - 1 \geq 0$.

At the same time, for $p \in (2k-1, 2k)$, this expression is strictly positive, because $\prod_{j=0}^{2k}(p - j) < 0$ and the monotone function $g_p(t) = (p-2k-1) - (p+d-2k-1)t$ takes values $g_p(0) = p - 2k - 1 < 0$ and $g_p(1) = -d < 0$. Thus, operator $D^{(k)}$ allows us to prove Propostion 1.4.3 for p in the range $(2k-1, 2k) \cup (2k, 2k+1]$. $\square$

We suspect that an analog of Theorem 1.1.3 also holds for the Fejes Tóth conjecture [51] mentioned in the introduction. Recall that this conjecture (its continuous version) deals with the energy I_f with potential $f(t) = \arcsin|t|$ and speculates that the discrete measure uniformly concentrated on the elements of an orthonormal basis minimizes I_f. If the conjecture is true, not all the minimizers of this energy are discrete. For example, as observed in [14], on $\mathbb{S}^3$, normalized uniform 1-dimensional Hausdorff measure on two orthogonal copies of $\mathbb{S}^1$, i.e. on the set

$$\{(x_1, x_2, 0, 0) : \, x_1^2 + x_2^2 = 1\} \cup \{(0, 0, x_3, x_4) : \, x_3^2 + x_4^2 = 1\},$$

would also yield a minimizer. This effect is related to the fact that, while the kernel $f(t) = \arcsin|t|$ is *not* positive definite on $\mathbb{S}^{d-1}$ with $d \geq 3$, it is indeed positive definite on $\mathbb{S}^1$, i.e. the uniform measure is a minimizer on the circle. Thus, assuming the conjecture, this energy does have non-discrete minimizers.

1.5 Minimizers of energies with analytic kernels

We can also prove a statement analogous to Theorem 1.1.3 for a wide class of energies – namely, those with analytic potentials.

Theorem 1.5.1. Assume that f is a real-analytic function on $[-1, 1]$, such that σ is not a minimizer of I_f, i.e. f is not (up to an additive constant) positive definite on $\mathbb{S}^{d-1}$. Let μ be a minimizer of I_f, then $(\mathrm{supp}(\mu))^\circ = \emptyset$. Moreover, when $d = 2$, then $\mathrm{supp}(\mu)$ must be discrete

Proof. Suppose, indirectly, that $(\mathrm{supp}(\mu))^\circ \neq \emptyset$. By Lemma 1.4.1, we know that the potential

$$F_\mu(x) = \int_{\mathbb{S}^{d-1}} f(\langle x, y \rangle) d\mu(y)$$

is constant on $\mathrm{supp}(\mu)$. Since $f(\langle x, y \rangle)$ is real-analytic on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$, $F_\mu(x)$ is real-analytic on $\mathbb{S}^{d-1}$. Since F_μ is real-analytic and constant on an open set in $\mathbb{S}^{d-1}$, it is constant on all of $\mathbb{S}^{d-1}$ [117, Lemma 2.4]. In addition, $F_\sigma(x) = I_f(\sigma)$ is constant on $\mathbb{S}^{d-1}$ due to rotational invariance. We then obtain

$$
\begin{aligned}
I_f(\mu) &= \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y\rangle) d\mu(y) d\mu(x) = \int_{\mathbb{S}^{d-1}} F_\mu(x) d\mu(x) = \int_{\mathbb{S}^{d-1}} F_\mu(x) d\sigma(x) \\
&= \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y\rangle) d\mu(y) d\sigma(x) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y\rangle) d\sigma(x) d\mu(y) \\
&= \int_{\mathbb{S}^{d-1}} F_\sigma(x) d\mu(y) = I_f(\sigma).
\end{aligned}
$$

This is clearly a contradiction, as by the assumption, I_f is not minimized by σ. Our first claim then follows.

For $\mathbb{S}^1$, we have that if F_μ is constant on a set $\{z_1, z_2, ...\} \subset \mathbb{S}^1$ with an accumulation point, F_μ is constant on $\mathbb{S}^1$. The proof of our second claim then follows as above. □

If $\mathbb{S}^{d-1}$ is replaced with one of the projective spaces $\mathbb{FP}^{d-1}$ ($\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, for instance) a similar result can be derived as above. In this case kernels f are also functions of the cosine of the geodesic distance $\tau(x, y) = 2|\langle x, y\rangle|^2 - 1$ under identification of points with unit vectors $x, y \in \mathbb{F}^d$; see Chapter 2 for more details on energy integrals over these spaces.

In the spirit of Theorem 1.5.1, as well as Corollary 1.2.5, it may be tempting to conjecture that if f (not necessarily analytic) is not positive definite on $\mathbb{S}^{d-1}$ (up to constant), i.e $I_f(\mu)$ is *not* minimized by σ, then the support of any minimizer of I_f must have empty interior. However, this is not true, as the following simple example shows. Assume that $f \in C[-1, 1]$ is constant near $t = 1$ and strictly decreasing otherwise, i.e. it satisfies for some fixed $\gamma \in (0, 1)$,

$$
f(1) = f(\tau) = \min_{t \in [-1,1]} f(t) \quad \text{for any} \quad \tau \in [1 - \gamma, 1],
$$

and $f(\tau) > f(1)$ for all $\tau \in [-1, 1 - \gamma)$. It is then evident that for any $z \in \mathbb{S}^{d-1}$

$$
\min_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) = I_f(\delta_z) = f(1),
$$

and $I_f(\sigma) > I_f(\delta_x)$, i.e. σ is not a minimizer of I_f. Let $C(z,\alpha) = \{x \in \mathbb{S}^{d-1} : \langle x, z\rangle > \alpha\}$ denote the *spherical cap* of "height" α centered at $z \in S^{d-1}$. Let ν be the normalized uniform measure on $C(z,\alpha)$, i.e.

$$d\nu(x) = \frac{\mathbf{1}_{C(z,\alpha)}(x)}{\sigma(C(z,\alpha))} d\sigma(x),$$

with $\alpha = 1 - \frac{\gamma}{4}$. Then for each $x, y \in C(z,\alpha)$, we have $\langle x, y\rangle > 1-\gamma$, and hence

$$I_f(\nu) = I_f(\delta_z) = f(1),$$

i.e. ν is also a minimizer of I_f, but its support has non-empty interior.

1.6 Applications of the results to energies with polynomial kernels

We observe that the results of Sections 1.3 and 1.5 apply if f is a polynomial. Indeed, Theorem 1.5.1 is applicable since polynomials are analytic, while the conditions of Theorem 1.3.3 hold because the Gegenbauer expansion has only finitely many terms. We summarize these statements in the following corollary.

Corollary 1.6.1. Assume that f is a polynomial whose Gegenbauer expansion is

$$f(t) = \sum_{n=0}^{m} a_n C_n^\lambda(t). \tag{1.6.1}$$

(i) There exists a discrete minimizer $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$ with

$$|\operatorname{supp}\mu| \le 1 + \sum_{\{n:\ a_n>0,\ 1\le n\le m\}} \dim \mathcal{H}_n^d.$$

(ii) If, moreover, σ is not a minimizer of I_f over $\mathcal{P}(\mathbb{S}^{d-1})$, i.e. there exists $n \ge 1$ such that $a_n < 0$, then the support of any minimizer of I_f has empty interior. For $\mathbb{S}^1$ the support is finite.

We observe that when $a_n > 0$ for $n = 1, \dots, m$, i.e. f is positive definite on $\mathbb{S}^{d-1}$ polynomial (up to constant), the statement of Theorem 1.3.3 (and hence also part (i) of the above corollary) is well known. In this case, the discrete minimizers $\mu = \sum \omega_{x_i} \delta_{x_i}$ are exactly *weighted spherical m-designs*, i.e. for any polynomial p of degree at most m we have

$$\sum_i \omega_{x_i} p(x_i) = \int_{\mathbb{S}^{d-1}} p(x) d\sigma(x).$$

A certain well-known generalization of this fact can also be easily deduced from part (i) of Corollary 1.6.1. Let $M \subset \mathbb{N}_0$ with $0 \in M$. Call a set $\{x_i\}_{i=1}^k \subset \mathbb{S}^{d-1}$ with positive weights ω_{x_i} a *weighted $\mathcal{M}$-design* if for every $m \in \mathcal{M}$ and for every spherical harmonic $Y \in \mathcal{H}_m^d$ one has

$$\sum_i \omega_{x_i} Y(x_i) = \int_{\mathbb{S}^{d-1}} Y(x) d\sigma(x).$$

When $\mathcal{M} = \{0, 1, \ldots, m\}$, this definition coincides with the definition of an m-design. Such objects arise naturally for some configurations. For example, the 600-cell, one of the six 4-dimensional convex regular polytopes with vertices which form a 120-point subset of $\mathbb{S}^3$, yields an exact cubature formula for spherical harmonics of degrees up to 19, *excluding* degree 12. In other words, it is an $\mathcal{M}$-design for $\mathcal{M} = \{0, 1, \ldots, 11\} \cup \{13, \ldots, 19\}$. By taking $a_n > 0$ only for $n \in \mathcal{M}$ and applying part (i) of Corollary 1.6.1, one easily concludes existence of weighted $\mathcal{M}$-designs on the sphere $\mathbb{S}^{d-1}$ of cardinality at most $\sum_{n \in \mathcal{M}} \dim \mathcal{H}_n^d$. This statement is encompassed by more general results [143, 123]

Theorem 1.3.3 and part (i) of Corollary 1.6.1 vastly generalize these well-known statements, essentially showing that the addition of any number of negative definite terms does not destroy the statement: discrete minimizers with the same cardinality still exist.

Concerning part (ii) of Corollary 1.6.1, it might be interesting to give some explicit examples of polynomials f with at least one negative coefficient $a_n < 0$ for $n \geq 1$, for which the minimizers of I_f are not necessarily discrete. Finally, we mention that the case of energy optimization for polynomial potentials in $d = 2$ is more approachable than in higher dimensions, due to the classical solution of the trigonometric moment problem [133, Theorem 1.4].

1.7 Local minimizers of the p-frame energy with $p \in 2\mathbb{N}$ are global.

Finally, we make an observation that for energies with positive definite kernels, including the p-frame energy with $p \in 2\mathbb{N}$, every local minimizer is necessarily global. We consider local minima in a rather general sense.

Definition 1.7.1. We say that a probability measure $\xi \in \mathcal{P}(\mathbb{S}^{d-1})$ is a local minimizer of I_f if for each $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$ and for any $\tau > 0$ small enough (depending on μ),

$$I_f(\xi) \leq I_f((1-\tau)\xi + \tau\mu).$$

Observe that this definition is satisfied if ξ is a local minimum with respect to many reasonable metrics on $\mathcal{P}(\mathbb{S}^{d-1})$, i.e. if there exists $\varepsilon > 0$ such that $I_f(\xi) \leq I_f(\mu)$ whenever $d(\xi, \mu) < \varepsilon$, where $d(\xi, \mu)$, represents, for example, the d_p-Wasserstein distance, $p < \infty$, or the total variation distance between measures. The following proposition provides a relation between the local and global minimizers.

Proposition 1.7.2. Let $f \in C[-1, 1]$ and let $\nu \in \mathcal{P}(\mathbb{S}^{d-1})$ be a global minimizer of I_f. Assume also that $\xi \in \mathcal{P}(\mathbb{S}^{d-1})$ is a local minimizer of I_f and that $\operatorname{supp} \xi \subset \operatorname{supp} \nu$. Then ξ is also a global minimizer of I_f over $\mathcal{P}(\mathbb{S}^{d-1})$.

If the function f is positive definite (modulo a constant term) on the sphere $\mathbb{S}^{d-1}$, then the uniform measure σ minimizes I_f according to part (iv) of Proposition 1.2.2, hence one can take $\nu = \sigma$ in the lemma above. Since σ is supported on the whole sphere, this immediately leads to non-existence of local minimizers which are not global:

Corollary 1.7.3. Let $f \in C[-1, 1]$ be positive definite on $\mathbb{S}^{d-1}$ (up to an additive constant) and let ξ be a local minimizer of I_f. Then ξ is necessarily a global minimizer of I_f, i.e.

$$I_f(\xi) = \min_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu).$$

Proof of Proposition 1.7.2. Let ν be a global minimizer, that is

$$I_f(\nu) = \inf_{\mu \in \mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) = \alpha.$$

According to Lemma 1.4.1, the potential of ν satisfies

$$F_\nu(x) = \int_{\mathbb{S}^{d-1}} f(\langle x, y \rangle) d\nu(y) = I_f(\nu) = \alpha \qquad \text{for all } x \in \operatorname{supp} \nu. \tag{1.7.1}$$

Suppose, by contradiction, that ξ satisfies $\alpha = I_f(\nu) < I_f(\xi)$. Since ξ is a local minimizer, setting $\mu_\tau = \tau\nu + (1-\tau)\xi$, for sufficiently small $0 < \tau < 1$, we have

$$I_f(\mu_\tau) \geq I_f(\xi). \tag{1.7.2}$$

Setting $I_f(\xi) = \beta > \alpha$ and using (1.7.1), a quick calculation shows that

$$\begin{aligned} I_f(\xi) \leq I_f(\mu_\tau) &= \tau^2 I_f(\nu) + (1-\tau)^2 I_f(\xi) + 2\tau(1-\tau) \int_{\mathbb{S}^{d-1}} F_\nu(x)\, d\xi(x) \\ &= \tau^2\alpha + (1-\tau)^2\beta + 2\tau(1-\tau)\alpha. \end{aligned}$$

Thus, $\tau^2\alpha + 2\tau(1-\tau)\alpha + (1-\tau)^2\beta \geq \beta$. However

$$\tau^2\alpha + 2\tau(1-\tau)\alpha + (1-\tau)^2\beta < \beta(\tau^2 + 2\tau(1-\tau) + (1-\tau)^2) = \beta,$$

which is a contradiction. □

Corollary 1.7.3 applies to the p-frame energies when $p = 2k$ is an even integer. As discussed in the introduction, σ minimizes I_f, since $f(t) = t^{2k}$ is positive definite. Thus, all the local minimizers of the $2k$-frame energy are necessarily global. A somewhat similar effect for $p = 2$ has been observed in [12] for discrete energies: it was proved that any finite configuration locally minimizing the N-point frame energy is also a minimizer, and therefore it is a tight frame, whenever $N \geq d$.[a]

[a]This chapter is adapted from the paper [15].

CHAPTER 2

OPTIMAL MEASURES FOR P-FRAME ENERGIES ON SPHERES

2.1 Introduction

An intriguing natural phenomenon is the ubiquitous appearance of certain symmetric structures and configurations as solutions to optimization problems. In a number of spaces, highly symmetric configurations of points such as the vertices of the icosahedron on $\mathbb{S}^2$ or the minimal vectors of the Leech lattice Λ_{24} on $\mathbb{S}^{23}$ are optimal codes [90]. First papers on t-designs made important connections between symmetry and optimality through pioneering work on linear programming bounds [44]. Some highly symmetric configurations, in addition to being t-designs and optimal codes, are also minimizers of harmonic energies [2, 81, 82, 161, 160].

For a finite configuration of points on the sphere, $\mathcal{C} \subset \mathbb{S}^{d-1}$, recall the definition of the discrete f-potential energy of $\mathcal{C}$ (as given in equation 1.1.1) and the definition of an *absolutely monotonic function*, a function with the property that all its derivatives on an interval are non-negative.

Universally optimal point configurations, i.e. collections of points $\mathcal{C}$ minimizing the discrete energies E_f among all point sets of fixed cardinality $|\mathcal{C}|$, for all absolutely monotonic functions f on $[-1, 1)$, are exceptional configurations discovered through the linear programming approach of Cohn and Kumar in [33].

As in the previous chapter, rather than considering configurations of fixed cardinality, we focus on the problem of minimizing energies over *all Borel probability measures*, discovering that surprisingly in many situations the minimizing measures are discrete again. For our potentials, the discrete energy for up to d particles is minimized by collections of orthogonal vectors. Since in this setting the energy does not change by replacing any x with λx, where $|\lambda|= 1$, its analysis naturally lends itself to the projective space $\mathbb{RP}^{d-1}$, where the potential becomes repulsive, and we adopt this approach in the technical parts of the paper.

The main examples of the above potentials, which motivate the current chapter, are of the form $f(t) = |t|^p$, $p > 0$, which yield the p-frame energies; see equation 1.1.4. As discussed in the previous chapter, this type of energy has a rich history.

Minimizers of this energy for $p = 2$ are precisely unit norm *tight frames*. These configurations, which explain the nomenclature "frame energy", play an important role in signal processing and other branches of applied mathematics and behave like overcomplete orthonormal bases. There are also other minimizers for $p = 2$, such as the surface area, or Haar measure σ on $\mathbb{S}_{\mathbb{F}}^{d-1}$, and, more generally, *isotropic probability measures* on the sphere, i.e. those measures for which

$$\int_{\mathbb{S}_{\mathbb{F}}^{d-1}} |\langle x, y\rangle|^2 d\mu(y) = \frac{1}{d}, \tag{2.1.1}$$

holds for all $x \in \mathbb{S}_{\mathbb{F}}^{d-1}$.

More generally, for even integers p, these energies were considered in earlier works [134, 154, 148], and it is known that for $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$ projective k-designs are precisely the finite configurations which minimize the $p = 2k$ energy. In this terminology, unit norm tight frames are equivalent to projective 1-designs (see Section 2.2.3 for precise definitions), while spherical 2-designs are exactly those unit norm tight frames, whose center of mass is at the origin. These were constructively shown to exist for $d \geq 2$ precisely when the number of points N satisfies $N \geq d + 1$ and $N \neq d + 2$ when d is odd [105]. The last restriction does not apply to unit norm tight frames, and these exist for all $N \geq d$ [12]. Surface measure is also known to be a minimizer for $p \in 2\mathbb{N}$: this can be seen from the fact that the function f is positive definite in this case (see Proposition 2.2.3), and was originally proved in the real case in [134].

For p not an even integer, optimal distributions of mass for p-frame energies are much less studied, to the point of there only being one result on these minimizing measures readily found in the literature (outsude of the results in the previous chapter). It states that distributing mass equally on the orthoplex or cross-polytope, an orthonormal basis and its antipodes, gives the unique symmetric minimizer, up to orthogonal transformations, for any energy with $p \in (0, 2)$ [50].

This result (contained in our Theorem 2.1.1 below as a special case) points to an interesting distinction. When p is even, the p-frame energy has a multitude of both continuous, e.g. σ, and discrete minimizers. However, this is not the case when p is not an even integer: σ is no longer a minimizer, since the function $f(t) = |t|^p$ is not positive definite, and so the above result, along with our numerical studies, points to existence of discrete minimizers only.

In this chapter we give a first description of minimizers for several dimensions and some ranges of p. The description relies on the notion of *tight designs*: designs of high strength, but with few distinct pairwise distances, see Definition 2.2.5. We show that if there exists a tight projective t-design (which in the real case is equivalent to a tight spherical $(2t+1)$-design), then it minimizes the p-frame energy for $p \in (2t-2, 2t)$. The 600-cell, despite not being a tight design, minimizes the p-frame energy for $p \in (8, 10)$ among probability measures on $\mathbb{S}^3$, as we show in Section 2.4.

Theorem 2.1.1. Let $f(t) = |t|^p$, $t \in [-1, 1]$.

(i) If there exists a tight spherical $(2t+1)$-design $\mathcal{C} \subset \mathbb{S}^{d-1}$, then the measure

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p-frame energy I_f with $2t - 2 \leq p \leq 2t$ over $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$.

(ii) Let $\mathbb{F} = \mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. Assume that there exists a tight projective t-design $\widetilde{\mathcal{C}} \subset \mathbb{FP}^{d-1}$, and let the code $\mathcal{C} \subset \mathbb{S}_{\mathbb{F}}^{d-1}$ consist of the representers of $\widetilde{\mathcal{C}}$ in $\mathbb{S}_{\mathbb{F}}^{d-1}$ according to (2.2.1). Then the measure

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p-frame energy I_f with $2t - 2 \leq p \leq 2t$ over $\mu \in \mathcal{P}(\mathbb{S}_{\mathbb{F}}^{d-1})$.

(iii) Let $\mathcal{C} \subset \mathbb{S}^3$ denote the 600-cell. Then the measure

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p-frame energy I_f with $8 \leq p \leq 10$ over $\mu \in \mathcal{P}(\mathbb{S}^3)$.

For parts (i)-(ii) of the above theorem we also prove a uniqueness statement: more precisely, whenever the corresponding statements hold, and additionally p is not an endpoint of the interval, i.e. $p \in (2t-2, 2t)$, *all* minimizers have to be tight designs (although not necessarily coinciding with $\mathcal{C}$), in particular, they have to be discrete. Since tight $(2t+1)$-designs on the circle consist just of $2(t+1)$ equally spaced points, the above result fully characterizes the minimizers for $d = 2$ (for both the sphere and real projective space). See Section 2.3.5 for more details.

We observe that part (i) is essentially contained in part (ii) with $\mathbb{F} = \mathbb{R}$: indeed, odd-strength tight spherical designs are necessarily symmetric, and by taking one point in each antipodal pair one obtains a tight projective design (see Sections 2.2.3–2.2.4 for a more extensive discussion).

Minimizing the continuous energy (1.1.4) over all *measures* and obtaining discrete minimizers allows us to make new conclusions about the minimizing configurations of the discrete energies (1.1.1) for certain values of the cardinality N. One directly obtains the following corollary:

Corollary 2.1.2. Let $\mathbb{F}$, d, p, and $\mathcal{C}$ be as in any of the parts of Theorem 2.1.1, and let $N = k|\mathcal{C}|$, $k \in \mathbb{N}$. Then N-point discrete p-frame energy is minimized by the configuration $\mathcal{C}$ repeated k times, i.e.

$$\min_{\substack{\mathcal{C}' \subset \mathbb{S}^{d-1}_{\mathbb{F}} \\ |\mathcal{C}'| = N}} \frac{1}{N^2} \sum_{x,y \in \mathcal{C}'} |\langle x, y\rangle|^p = I_{|t|^p}\Big(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x\Big). \tag{2.1.2}$$

Thus, for example, if N is a multiple of 6, then repeated copies of a “half” of the icosahedron minimize the N-point p-frame energy on $\mathbb{S}^2$ for $p \in [2, 4]$.

The arguments proving Theorem 2.1.1 are based on the linear programming method which goes back to Delsarte and Yudin [45, 161] and are reminiscent of those appearing in [33]. Theorem 2.1.1 is a consequence of a much more general statement, Theorem 2.3.7. The latter theorem, in fact, demonstrates that tight t-designs possess a certain *universality* property: they minimize the energy *for all* strictly monotonic functions of degree exactly t over *all probability measures*, see Section 2.3 for details.

The proof of optimality for the 600-cell is computer assisted and makes use of the fact that the averages of spherical harmonics over the 600-cell vanish for a few orders above its maximal degree as a spherical design – the same idea was used in the proof of universal optimality of the 600-cell in [33], as well as earlier in [2, 1]. This allows us to construct a collection of interpolating polynomials h for each p which have the desired properties of lying below f, agreeing with f on the distances appearing in $\mathcal{C}$, and finally being positive definite, the last of which is checked using interval arithmetic. The details of the proof are taken up in Section 2.4.

We collect all the necessary preliminary material in Section 2.2: Section 2.2.1 contains the discussion of relevant properties of compact 2-point homogeneous connected spaces; Section 2.2.2 explains the specifics of minimizing energy functionals over probability measures on such spaces; Section 2.2.3 introduces designs, and, in particular, tight designs; and Section 2.2.4 describes the transference between energies on projective spaces and spheres, which connects Theorem 2.3.7 to Theorem 2.1.1.

Extensive numerical experiments were conducted in the course of our investigations. The results of these experiments are collected in Table 2.1 for the real case and Table 2.2 for the complex case. Unlike the case of tight designs, optimal weights for these configurations are generally not equal and thus must be computed for each relevant value of p. Each table gives the minimal support size of a conjectured optimal point set: when a configuration on the sphere is origin-symmetric, this minimal support size equals half of the size of the named configuration. For example, the icosahedron has twelve vertices, however 6 vertices on one hemisphere suffice to give a minimizer of the 3-frame energy on $\mathbb{S}^2$. We give additional details in Section 2.5 for these conjectured minimizers of the p-frame energies. Notably several of these configurations are not universally optimal, and further, several universally optimal configurations are nowhere to be found in this table. We discuss common features of minimizers in Section 2.9. More details on symmetry of measures and relations between spheres and projective spaces may be found in Section 2.2.4.

Our experimental results together with Theorem 2.1.1 further support Conjecture 1.1.1 from the previous chapter, namely that clustering of minimizers is a general phenomenon when p is not an even integer.

In addition to the conjectured discreteness of minimizers our initial study gave rise to surprisingly symmetric minimizers for p-frame energies, suggesting that further investigation might give new interesting spherical codes. While nearly all of the minimizing configurations arising from our numerical experiments have appeared before in the coding theory literature, we did however discover a new code in $\mathbb{C}^5$ of 85 vectors which in turn gives a new bound for a minimal sized weighted projective 3-design. We detail a construction of this code and its properties in Section 2.5.1.

Section 2.6 extends some of our results to non-compact settings. In Section 2.7 we apply the results of Theorem 2.1.1 to the problems of minimizing mixed volumes of convex bodies, and in Section 2.8 we apply the methods of linear programming, similar to those employed in Theorems 2.1.1 and 2.3.7, to the optimization of other kernels, motivated in part by questions from mathematical physics, see [53].

We would like to point out that in many papers, the term *p-frame potential* is usually used to denote the p-frame energy (1.1.4) or its discrete counterpart. We find the term "energy" to be more appropriate in this context and reserve the term "potential" for the kernel $f(t)$ of the energy I_f.

2.2 Geometry and functions on 2-point homogeneous spaces

2.2.1 Two-point homogeneous spaces

For convenience, the above discussion mostly assumed the underlying space to be the unit sphere $\mathbb{S}^{d-1}$. This will no longer be the case, as our study concerns energy minimization on a broader class of spaces. A metric space (Ω, d) is said to be *two-point homogeneous*, if for every two pairs of points x_1, x_2 and y_1, y_2 such that $d(x_1, x_2) = d(y_1, y_2)$ there exists an isometry of Ω, mapping x_i to y_i, $i = 1, 2$. It is known [153] that any such compact connected space is either a real sphere $\mathbb{S}^{d-1}$, a real projective space $\mathbb{RP}^{d-1}$, a complex projective space $\mathbb{CP}^{d-1}$, a quaternionic projective space $\mathbb{HP}^{d-1}$, or the Cayley projective plane $\mathbb{OP}^2$. Note that it suffices to consider $\mathbb{FP}^{d-1}$ for $d > 2$ only, as $\mathbb{FP}^1$ is just $\mathbb{S}^{\dim_{\mathbb{R}} \mathbb{F}}$ [4, p. 170], and so will not be separately considered in what follows.

Below, Ω always refers to a compact connected 2-point homogeneous space, equipped with the geodesic distance ϑ, normalized to take values in $[0, \pi]$. We let σ denote the unique probability measure invariant under the isometries of Ω.

The first three types of projective spaces $\{\mathbb{FP}^{d-1} : \mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}\}$ have a simple description: they may be represented as the spaces of lines passing through the origin in $\mathbb{F}^d$,

$$x\mathbb{F} = \{x\lambda \mid \lambda \in \mathbb{F} \setminus \{0\}\}. \tag{2.2.1}$$

Observe that the isometry groups $O(d)$, $U(d)$, $Sp(d)$ of the corresponding vector spaces $\mathbb{F}^d$ act transitively on each space, and that the stabilizers of a line represented by $x \in \mathbb{F}^d$ are $O(d-1)\times O(1)$, $U(d-1) \times U(1)$, and $Sp(d-1) \times Sp(1)$, respectively. Thus one has [157, p. 28] the following quotient representations:

$$\mathbb{RP}^{d-1} = O(d)/O(d-1) \times O(1),$$
$$\mathbb{CP}^{d-1} = U(d)/U(d-1) \times U(1),$$
$$\mathbb{HP}^{d-1} = Sp(d)/Sp(d-1) \times Sp(1),$$

where we write $O(d)$, $U(d)$, $Sp(d)$ for the groups of matrices X over the respective algebra, satisfying $XX^* = I$.

Using the identification (2.2.1), one can associate each element of $\mathbb{FP}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$) with a unit vector $x \in \mathbb{F}^d$, $\|x\|= 1$, and we shall often abuse notation by doing so. This gives, in addition to the Riemannian metric ϑ, another metric, the *chordal distance* between points $x, y \in \Omega$, defined by

$$\rho(x, y) = \sqrt{1 - |\langle x, y\rangle|^2},$$

where $\langle x, y\rangle = \sum_{i=1}^{d} x_i\overline{y}_i$ is the standard inner product in $\mathbb{F}^d$. The chordal distance $\rho(x, y)$ is related to the geodesic distance $\vartheta(x, y)$ by the equation

$$\cos\vartheta(x, y) = 1 - 2\rho(x, y)^2 = 2|\langle x, y\rangle|^2-1.$$

Since the algebra of octonions is not associative, the line model of (2.2.1) fails, and instead a model given by Freudenthal [58] is used to describe $\mathbb{OP}^{d-1}$. It is known [4] that only two octonionic spaces exist: $\mathbb{OP}^1$ and $\mathbb{OP}^2$, however $\mathbb{OP}^1$ is just $\mathbb{S}^8$, as noted above.

$\mathbb{OP}^2$ can be described as the subset of 3×3 Hermitian matrices Π over $\mathcal{O}$, satisfying $\Pi^2 = \Pi$ and Tr $\Pi = 1$ [135]. A metric for $\mathbb{OP}^2$ is then given by the Frobenius product,

$$\rho(\Pi_1, \Pi_2) = \frac{1}{\sqrt{2}} \|\Pi_1 - \Pi_2\|_F = \sqrt{1 - \langle \Pi_1, \Pi_2 \rangle},$$

where $\langle \Pi_1, \Pi_2 \rangle = \text{Re Tr } \frac{1}{2}(\Pi_1 \Pi_2 + \Pi_2 \Pi_1)$. This is the chordal distance on $\mathbb{OP}^2$ whereas the geodesic distance can be defined through $\sin \frac{\vartheta(x,y)}{2} = \rho(x, y)$, as in the above projective spaces. All Π given as above may be written in the form

$$\begin{pmatrix} |a|^2 & a\bar{b} & a\bar{c} \\ b\bar{a} & |b|^2 & b\bar{c} \\ c\bar{a} & c\bar{b} & |c|^2 \end{pmatrix},$$

where $|a|^2 + |b|^2 + |c|^2 = 1$ and $(ab)c = a(bc)$. This gives a representation of $\mathbb{OP}^2$ as the quotient $F_4/\text{Spin}(9)$ [4, p. 189].

One feature of spaces Ω that allows for the application of linear programming methods is the existence of a decomposition of $L^2(\Omega, \sigma)$, the space of complex-valued square-integrable functions on Ω, into irreducible representations:

$$L^2(\Omega, \sigma) = \bigoplus_{n \geq 0} V_n,$$

where spaces V_n are finite-dimensional and invariant under the isometries of Ω (see [90]). Moreover, they can be chosen as the eigenspaces of the Laplace–Beltrami operator on Ω corresponding to the n-th eigenvalue in the increasing order. Let $Y_{n,k}$, $k = 1, \ldots, \dim V_n$, be an orthonormal basis in V_n. Because of the invariance of V_n and due to the two-point homogeneity of Ω, the reproducing kernel for V_n only depends on the distance $\vartheta(x, y)$ between points [148]. Furthermore, as a function of

$$\tau(x, y) := \cos\vartheta(x, y).$$

the reproducing kernel is a polynomial C_n of degree n, which satisfies

$$C_n(\tau(x, y)) = \frac{1}{\dim V_n} \sum_{k=1}^{\dim V_n} Y_{n,k}(x)\overline{Y_{n,k}(y)}. \tag{2.2.2}$$

Formula (2.2.2) is the general form of the *addition formula*, and shows that functions C_n are *positive definite* on Ω, that is,

$$\sum_{1 \le i,j \le k} c_i \bar{c}_j C_n(\tau(x_i, x_j)) \ge 0$$

for all coefficients $\{c_i\}_{i=1}^k \subset \mathbb{F}$, and all vectors $\{x_i\}_{i=1}^k \subset \Omega$.

The polynomials C_n given in (2.2.2) satisfy $C_n(1) = 1$ and are orthogonal with respect to the probability measure

$$d\nu^{(\alpha,\beta)} = \frac{1}{\gamma_{\alpha,\beta}}(1-t)^\alpha(1+t)^\beta dt,$$

where $\alpha = (d-1)\dim_{\mathbb{R}}(\mathbb{F})/2 - 1$ and

$$\beta = \begin{cases} \alpha, & \text{if } \Omega = \mathbb{S}^{d-1}; \\ \dim_{\mathbb{R}}(\mathbb{F})/2 - 1, & \text{if } \Omega = \mathbb{FP}^{d-1}, \end{cases} \tag{2.2.3}$$

and the normalization factor is given by

$$\gamma_{\alpha,\beta} = 2^{\alpha+\beta+1}B(\alpha+1, \beta+1),$$

where B is the beta function. Jacobi polynomials form an orthogonal basis in $L^2([-1, 1], d\nu^{(\alpha,\beta)})$; equivalently, the span of $C_n(\tau(x, y))$, $n \ge 0$, is dense in the subset of $L^2(\Omega \times \Omega, \sigma \otimes \sigma)$ consisting of functions that depend only on the distance between x and y.

This allows expanding functions from $L^2([-1,1], d\nu^{(\alpha,\beta)})$ in terms of C_n (this generalizes the expansion in equation 1.2.2 to the other spaces):

$$f(t) = \sum_{i=0}^{\infty} \widehat{f}_n C_n(t), \quad \text{where} \quad \widehat{f}_n = \dim V_n \int_{-1}^{1} f(t) C_n(t)\, d\nu^{(\alpha,\beta)}(t).$$

As we have already done above, for a fixed space Ω we will not indicate the dependence of polynomials $C_n = C_n^{(\alpha,\beta)}$ on the indices α, β. We refer to $\widehat{f}_n$ as the Jacobi coefficients of the function f; the normalization $C_n(1) = 1$ used here is common in the coding theory community [141, 90].

2.2.2 Energies on 2-point homogeneous spaces

For the space of probability measures $\mathcal{P}(\Omega)$ supported on Ω, and for a lower semi-continuous function $f : [-1,1] \to \mathbb{R} \cup \infty$, the f-energy integral is defined as the functional mapping μ to

$$I_f(\mu) = \int_{\Omega}\int_{\Omega} f(\tau(x,y)) d\mu(x) d\mu(y).$$

Observe that when $\Omega = \mathbb{S}^{d-1}$, we have $\tau(x,y) = \cos\vartheta(x,y) = \langle x, y\rangle$ and the definition above coincides with (1.1.2).

The notion of positive definiteness introduced in the previous chapter (see equation 1.2.1) naturally generalizes to the other spaces, and this notion plays heavily in the derivation of linear programming bounds we use to obtain our main results. Below $C[-1,1] = C_{\mathbb{R}}[-1,1]$ denotes the space of continuous real valued functions on the interval $[-1,1]$.

Definition 2.2.1. Let $f \in C[-1,1]$. We say that f is *positive definite* on Ω if for any set $\{x_1, \ldots, x_N\} \subset \Omega$ the matrix $[f(\tau(x_i, x_j))]_{i,j=1}^N$ is positive semidefinite, i.e. for every collection $\{c_1, \ldots, c_k\} \subset \mathbb{C}$ we have

$$\sum_{1 \le i,j \le N} f(\tau(x_i, x_j)) c_i \overline{c_j} \ge 0.$$

We have already seen that the Jacobi polynomials C_n are positive definite on Ω, and so their positive linear combinations must also be. This implication can be reversed, as contained in Proposition 1.2.2 for the spherical case. This fact holds generally for our compact 2-point homogeneous spaces.

Proposition 2.2.2. [18, 129, 62] A function $f \in C[-1,1]$ is positive definite on Ω if and only if $\widehat{f}_n \geq 0$ for all $n \geq 0$.

The fact that positive definite functions f give rise to f-energy integrals which are minimized over probability measures by the surface (or Haar) measure σ on Ω also adapts to this setting. This result appears in a number of papers, see for instance [41, 13]. We adapt the proof given in [13] to our purposes, choosing to work with the real and imaginary parts of the functions $Y_{n,k}$ defined above. By a slight abuse of notation, we use the same notation for these functions.

Proposition 2.2.3. Let $f \in C[-1,1]$, $f(t) = \sum\limits_{n=0}^{\infty} \widehat{f}_n C_n(t)$, and $\mu \in \mathcal{P}(\Omega)$. Then, the following are equivalent:

(i) $\widehat{f}_n \geq 0$ for all $n \geq 1$,

(ii) the surface measure σ is a minimizer of $I_f(\mu)$.

Moreover, σ is the unique minimizer of $I_f(\mu)$ if and only if $\widehat{f}_n > 0$ for all $n \geq 1$.

To prove this statement we use the following lemma, generalizing the behavior of Fourier expansions with positive coefficients [62, 97] to Jacobi expansions with the same property.

Lemma 2.2.4. Let $f \in C[-1,1]$, $f(t) = \sum\limits_{n=0}^{\infty} \widehat{f}_n C_n(t)$, and $\widehat{f}_n \geq 0$ for all $n \geq 1$. Then the Jacobi expansion of f converges uniformly and absolutely to f on $[-1,1]$.

Proof of Proposition 2.2.3. We first show that σ is a minimizer of $I_f(\mu)$. Assume that $\widehat{f}_n \geq 0$ for all $n \geq 1$. Then by the lemma above, the Fubini theorem, and the addition formula, we have

$$\begin{aligned} I_f(\mu) &= \sum_{n=0}^{\infty} \widehat{f}_n \int_\Omega \int_\Omega C_n(\tau(x,y)) d\mu(x) d\mu(y) \\ &= \sum_{n=0}^{\infty} \widehat{f}_n \cdot \frac{1}{\dim V_n} \sum_{n=1}^{\dim V_n} \int_\Omega \int_\Omega Y_{n,k}(x) Y_{n,k}(y) d\mu(x) d\mu(y) \\ &= \widehat{f}_0 + \sum_{n=1}^{\infty} \frac{1}{\dim V_n} \cdot \widehat{f}_n b_{n,\mu}, \\ &\geq \widehat{f}_0 = I_f(\sigma). \end{aligned}$$

The last inequality holds since $b_{n,\mu} = \sum_{k=1}^{\dim V_n} \left[\int_\Omega Y_{n,k}(x) d\mu(x) \right]^2 \geq 0$. If $\widehat{f}_n > 0$ for all $n \geq 1$, then equality can be achieved above only if μ is orthogonal to all spaces V_n, which directly implies that $\mu = \sigma$. If $\widehat{f}_n < 0$ for some $n \geq 1$, then set $d\mu(x) = (1 + \epsilon Y_{n,1}(x)) d\sigma(x)$, where $\epsilon > 0$ is sufficiently small so that $(1 + \epsilon Y_{n,1}(x)) \geq 0$ on Ω. Orthogonality and the addition formula (or Funk-Hecke formula) give that for $Y \in \mathcal{H}_n$,

$$\int_\Omega f(\tau(x,y)) Y(x) d\sigma(x) = \widehat{f}_n Y(y) \text{ and } \int_\Omega Y_{n,1}(x) d\sigma = 0.$$

Thus,

$$\begin{aligned} I_f(\mu) &= \int_\Omega \int_\Omega f(\tau(x,y))(1 + \epsilon Y_{n,1}(x))(1 + \epsilon Y_{n,1}(y)) d\sigma(x) d\sigma(y) \\ &= I_f(\sigma) + \epsilon^2 \widehat{f}_n \int_\Omega Y_{n,1}^2(x) d\sigma(x) < I_f(\sigma), \end{aligned}$$

implying that σ is not a minimizer for $I_f(\mu)$. If $\widehat{f}_n = 0$ for some $n \geq 1$, the same argument shows that $I_f(\mu) = I_f(\sigma)$, i.e. σ is not the unique minimizer. $\square$

The p-frame energies correspond to taking $\Omega = \mathbb{FP}^{d-1}$ ($\mathbb{F} = \mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$) and f of the form

$$f(t) = \left(\frac{1+t}{2} \right)^{\frac{p}{2}}, \tag{2.2.4}$$

because in this case, since $\tau(x,y) = \cos\vartheta(x,y) = 2|\langle x,y\rangle|^2 - 1$, we have

$$f(\tau(x,y)) = f(2|\langle x,y\rangle|^2 - 1) = |\langle x,y\rangle|^p.$$

We shall now prove that, whenever p is an even integer, these energies are minimized by the uniform measure on Ω.

When $p = 2k$ and $\Omega = \mathbb{FP}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}$, or $\mathbb{H}$), we have that $f(t) = 2^{-k} \cdot (1+t)^k$ is a polynomial. It is standard to check that this polynomial is positive definite on Ω: this could be done by checking that the coefficients in its Jacobi expansion are non-negative, but it would be perhaps simpler to prove it as follows. Observe that, since $C_0^{(\alpha,\beta)}(t) = 1$ and $C_1^{(\alpha,\beta)}(t) = \frac{\alpha-\beta}{2(\alpha+1)} + \frac{\alpha+\beta+2}{2(\alpha+1)} \cdot t$, we have that

$$1 + t = \frac{2(\alpha+1)}{(\alpha+\beta+2)}\, C_1^{(\alpha,\beta)}(t) \,+\, \frac{2(\beta+1)}{\alpha+\beta+2}\, C_0^{(\alpha,\beta)}(t).$$

Since $\alpha + 1 = \frac{d-1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$ and $\beta + 1 = \frac{1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$, we see that the function $1+t$ is positive definite on Ω. The well known Schur's theorem on Hadamard (elementwise) products of positive semidefinite matrices implies that if g and h are positive definite on Ω, then so is their product gh, and, in particular, all integer powers g^n are positive definite. Hence, the function $f(t) = 2^{-k} \cdot (1+t)^k$ is positive definite on Ω, and therefore $I_f(\sigma)$ is minimized by the uniform surface measure σ.

The minimal values of the $p = 2k$ energy may be expressed in elementary functions for each $\mathbb{F}$. These constants, $c_{\mathbb{F}}(d,k)$, are given below

$$\begin{aligned}
c_{\mathbb{F}}(d,k) &= \frac{1 \cdot 3 \cdot 5 \ldots (2k-1)}{d \cdot (d+2) \ldots (d+2(k-1))}, && \mathbb{F} = \mathbb{R},\\
c_{\mathbb{F}}(d,k) &= 1 \Big/ \binom{d+k-1}{k}, && \mathbb{F} = \mathbb{C},\\
c_{\mathbb{F}}(d,k) &= (k+1) \Big/ \binom{2d+k-1}{k}, && \mathbb{F} = \mathbb{H}.
\end{aligned}$$

When p is not an even integer, the p-frame energies are not positive definite, due to the appearance of negative terms in the Jacobi polynomial expansion of f, hence σ does not minimize the p-frame energy for $p \notin 2\mathbb{N}$.

2.2.3 Designs

We now treat the topic of designs in the compact connected two-point homogeneous spaces Ω. A finite set $\mathcal{C} \subset \Omega$ is called a *t-design* if

$$\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} p(x) = \int_{\Omega} p(x)\, d\sigma_{\Omega}(x) \tag{2.2.5}$$

holds for all polynomials p of degree at most t. Here $d\sigma_{\Omega}(x)$ is the Haar (or surface) measure on Ω. A relaxation of the above identity allows the configuration to be weighted, so that the equality

$$\sum_{x \in \mathcal{C}} \omega_x p(x) = \int_{\Omega} p(x)\, d\sigma_{\Omega}(x), \tag{2.2.6}$$

holds for some weights $\{\omega_x\}_{x \in \mathcal{C}} \subset \mathbb{R}_{\geq 0}$, satisfying $\sum_{x \in \mathcal{C}} \omega_x = 1$, and all polynomials p of degree at most t. Such weighted formulas are called *cubature formulas* or *weighted designs*. In both of the above equations, it is understood that polynomials p may be given explicitly as complex-valued functions which are polynomials in coordinates of $\mathbb{F}^d$, satisfying additionally $p(\alpha x) = p(x)$, for $|\alpha| = 1$, $\alpha \in \mathbb{F}$, in the projective case.

The *strength* of a (weighted) design is the maximum value of t for which identity (2.2.5) (accordingly, (2.2.6)) holds. A t-design can be equivalently defined as a configuration $\mathcal{C} \subset \Omega$, for which

$$\sum_{x,y \in \mathcal{C}} C_n(\tau(x,y)) = 0 \quad \text{for } 1 \leq n \leq t.$$

Similarly, $\mathcal{C}$ is a t-design in Ω if and only if it satisfies

$$\sum_{x \in \mathcal{C}} Y(x) = 0 \ \text{ for } Y \in \bigoplus_{n=1}^{t} V_n.$$

Linear programming bounds imply exact constraints on the size of *tight designs*, configurations which, in addition to being t-designs, have the smallest possible number of pairwise distances between their elements, for a design of strength t. The exact definition may be given as follows.

Definition 2.2.5. A discrete set $\mathcal{C} \subset \Omega$ is called a *tight t-design* if one of the following conditions is satisfied.

(i) $\mathcal{C}$ is a design of degree $t = 2m - 1$ and there are m distances between its distinct elements, including at least one pair diameter apart;

(ii) $\mathcal{C}$ is a design of degree $t = 2m$ and there are m distances between its distinct elements.

Tight spherical 2-designs are precisely regular simplices. For $d \geq 3$ and $t \geq 4$ there are eight tight spherical designs known. Tight odd-degree spherical designs must be centrally symmetric [44], and by choosing points from each antipode in an odd tight design one arrives at a real projective tight design. Six of the eight designs mentioned above are odd degree and correspond to the first six entries in the Table 2.3. The (remaining) known tight spherical 4-designs are the Schläfli configuration of 27 points in $\mathbb{S}^5$ and the 275 point arrangement associated with the McLaughlin group in $\mathbb{S}^{21}$.

Tight spherical designs with $d \geq 3$ and $t \geq 4$ may only exist for $t = 4, 5$, and 7 with the one exception of the spherical 11-design formed by the Leech lattice minimal vectors [7, 8]. The problem of finding tight spherical 5-designs is the same as that of finding maximal equiangular tight frames, and it is known that existence of a tight spherical 5-design in $\mathbb{S}^{d-1}$ is possible only for $d = 1, 2, 3$, and for dimensions of the form $d = (2k+1)^2 - 2$, where $k \geq 1$; see [10] for details on how these conditions arise. A direct correspondence with such spherical designs and regular graphs has long been recognized [131], and in connection, it is known that for $d = 47$ a tight spherical 5-design cannot exist [98]. For projective spaces, it is known that no tight t-designs exist in the complex or quaternionic setting whenever $t \geq 4$ and $d \neq 2$ [9, 72, 97]. With exception of the $(3, 15)$ quaternionic and $(3, 27)$ octonionic designs from [34], explicit constructions are readily found in the literature for the designs mentioned in Table 2.3.

A weaker property of a design is sharpness, which will not play a role here. The paper [33] proves that sharp designs, and tight designs in particular, are minimizers for discrete minimization problems with absolutely monotone kernels. A similar approach allows us to show that tight designs are optimal for the continuous p-frame energy.

2.2.4 Antipodal symmetry

We observe that the energy I_f on the sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$ for the kernels f with $f(t) = f(|t|)$ remains the same after averaging over unit multiples of vectors in the support of μ. Let $U(\mathbb{F})$ be the set of units in $\mathbb{F}$, $U(\mathbb{F}) = \{c \in \mathbb{F} \mid |c| = 1\}$, and η be the uniform measure on $U(\mathbb{F})$. If one defines, for Borel sets $B \subset \mathbb{S}_{\mathbb{F}}^{d-1}$,

$$\nu(B) = \frac{1}{\eta(U_{\mathbb{F}})} \int_{U_{\mathbb{F}}} \mu(cB) d\eta(c),$$

then $I_f(\nu) = I_f(\mu)$ for potential functions f as above. This is the primary reason it is natural to consider projective spaces $\mathbb{FP}^{d-1}$ as the optimization spaces for p-frame energies, as opposed to the spheres, in the cases when the elements $x \in \mathbb{FP}^{d-1}$ may be represented by unit vectors in $\mathbb{F}^d$.

This discussion shows that a minimizing measure on the sphere for $I_f(\mu)$, with f as above, can be taken to be symmetric, and that the problem of minimizing over symmetric measures on spheres is equivalent to minimizing energy over projective spaces. In particular, this explains part (i) of Theorem 2.1.1, since tight spherical $(2t+1)$-designs are necessarily symmetric and hence correspond to tight real projective t-designs.

As a final discussion point on the form of our energies, note that the kernel $f(t) = (\frac{1+t}{2})^{\frac{p}{2}}$ has as first negative derivative $f^{(\lceil p/2 \rceil + 1)}(t)$, $-1 < t < 1$. This plays an important role in what follows and it is precisely functions with this property of alternating derivative sign (for a large enough index) which our results apply to.

2.3 Optimality of tight designs for kernels absolutely monotonic to degree M

2.3.1 Linear programming

The main goal of this section is to show that for those dimensions and values of t for which tight designs exist, they are the global minimizers of the p-frame energies for intervals of p between consecutive even integers. We will use linear programming bounds to this end.

The linear programming method provides bounds for optima in various optimization problems, and its use is often aided by computational tools, where a problem is approximated by a finite-dimensional or discretized counterpart, then solved with a computer. It is surprising that this simple method provides optimal bounds often. This technique applies to all the compact 2-point homogeneous spaces Ω described above.

Our application of the method can be summed up in the following lemma, which is a measure-theoretic counterpart of the linear programming bound of Delsarte and Yudin [45, 161].

Lemma 2.3.1. Let $h \in C[-1,1]$ be a positive-definite function, i.e. $h(t) = \sum\limits_{n=0}^{\infty} \widehat{h}_n C_n(t)$ and $\widehat{h}_n \geq 0$ for all $n \geq 0$.

(i) Assume that $h(t) \leq f(t)$ for all $t \in [-1,1]$, then for any $\mu \in \mathcal{P}(\Omega)$,

$$I_f(\mu) \geq \widehat{h}_0 = I_h(\sigma).$$

(ii) Assume further that h is a polynomial of degree k and that there exists a k-design $\mathcal{C} \subset \Omega$ such that $h(t) = f(t)$ for each $t \in \{\tau(x,y) :\ x, y \in \mathcal{C}\}$. Then for any $\mu \in \mathcal{P}(\Omega)$,

$$I_f(\mu) \geq I_f\Big(\frac{1}{|\mathcal{C}|}\sum_{x\in\mathcal{C}} \delta_x\Big),$$

i.e. I_f is minimized by the uniform distribution on $\mathcal{C}$.

Proof. For the first part observe that

$$I_f(\mu) \geq I_h(\mu) \geq I_h(\sigma) = \widehat{h}_0,$$

where the first inequality follows from the fact that $f \geq h$, while the second one is due to Proposition 2.2.3, since h is positive definite.

For the second part, one can continue as follows

$$I_h(\sigma) = I_h\Big(\frac{1}{|\mathcal{C}|}\sum_{x\in\mathcal{C}} \delta_x\Big) = I_f\Big(\frac{1}{|\mathcal{C}|}\sum_{x\in\mathcal{C}} \delta_x\Big).$$

The first equality follows from the fact that $\mathcal{C}$ is a k-design, and the second one from the fact that f and h coincide on the set $\{\tau(x,y) :\ x, y \in \mathcal{C}\}$. Together with part (i) this proves the statement in part (ii). $\square$

This lemma provides insights in two different ways for how the linear programming method can be applied.

If a candidate $\mathcal{C}$ is available, one can apply part (ii) of Lemma 2.3.1 by constructing a polynomial $h \leq f$ as a Hermite interpolant of the function f at the points of $\{\tau(x,y) :\ x, y \in \mathcal{C}\}$. This reasoning, which lies behind the proof of Theorems 2.3.7 and 2.1.1, explains the appearance of tight designs: indeed, the number of elements in the set of interpolation points (i.e. distinct distances between the points of $\mathcal{C}$) determines the degree of the interpolant h – hence one wants a design of high strength, but with few mutual distances.

The same reasoning as above applies to the emergence of sharp designs as universally optimal sets in [33], and it also explains why this slightly weaker notion does not suffice for our purposes: since we are working with general measures rather than point sets with fixed cardinality, we cannot avoid interpolating at the point $t = 1$, which requires a design of higher strength. The main technical difficulty in this setting is proving positive definiteness of the Hermite interpolating polynomial h. We take this approach to Theorem 2.3.7 and carry out the technicalities in Sections 2.3.2–2.3.4.

If a suitable candidate is not available, one can still rely on part (i) of Lemma 2.3.1 and attempt to optimize the value of the energy $I_h(\sigma)$ over auxiliary positive definite polynomials h, obtaining a lower bound for the energy over all probability measures. If the degree of an auxiliary function h is bounded by D, we have $D+1$ non-negative variables $\widehat{h}_i$, $0 \leq i \leq D$, and infinitely many linear constraints $h(t) \leq f(t)$ for all $t \in [-1, 1]$. In order to get the best possible lower bound, we need to maximize $\widehat{h}_0$ given these linear conditions.

This problem is, generally, intractable as a linear optimization problem. However, when f is a polynomial, the condition $f(t) - h(t) \geq 0$ for all $t \in [-1, 1]$ may be represented as a finite-size positive semi-definite constraint on the coefficients $\widehat{h}_i$. In particular, the polynomial inequality may be rewritten as a sum-of-squares optimization problem (see, for instance, [112]) and thus solved as a semi-definite program.

By using sum-of-squares optimization described above, we obtain lower bounds on the p-frame energies over measures on projective spaces when p is an odd integer. A table of such bounds for real projective spaces $\mathbb{RP}^{d-1}$, $3 \leq d \leq 24$, and $p = 3, 5, 7$, is shown in Table A.2 in the Appendix. The concrete bounds are computed by a series of steps. For the first step, we fix the degree D of the auxiliary polynomial and solve the sum-of-squares problem. The numerical solver outputs a polynomial which is feasible up to a small tolerance. By rounding coefficients, it is then possible to obtain polynomials which are less than f and positive definite.

Since the choice of the maximal degree D is arbitrary, not much is lost by rounding, and our bounds in the appendix are thus rounded down to four significant figures. The last condition $f - h \geq 0$ can be checked using interval arithmetic, or by hand in simple cases. We include the coefficients of the auxiliary polynomials in the appendix. The polynomials used for $p = 3$ and $p = 5$ are of degree $D = 6$, while the polynomials for $p = 7$ are of degree $D = 8$.

It is interesting to compare the values of conjectured energy minimizers with the lower bounds obtained using the approach above. We make comparison of these bounds in Table 2.4 below for all conjectured optimizers from Tables 2.1 and 2.2: observe that the values are indeed close, which motivates our conjectures about the minimizers. Tight designs are excluded from this table since for them the lower and the upper bounds coincide as we will show below in Theorem 2.3.7.

2.3.2 Properties of orthogonal polynomials

As already pointed out, for fixed Ω, we write simply $C_n(t) = C_n^{(\alpha,\beta)}(t)$. Recall that $C_n(1) = 1$. In some of the arguments in Section 2.3.4 we will use instead the monic polynomials proportional to C_n; we therefore introduce notation $Q_n(t) = Q_n^{(\alpha,\beta)}(t)$ for these Jacobi polynomials.

In this subsection we collect several results about orthogonal polynomials relevant to the proof of our main theorem. Fix a space Ω, and let α and β be the corresponding parameters of the associated Jacobi polynomials. According to Proposition 2.2.3, a function being positive definite on Ω is equivalent to having positive coefficients in the Jacobi expansion in terms $Q_n^{(\alpha,\beta)}$.

It will be useful to consider *adjacent* Jacobi polynomials, defined as one of the three sequences $Q_n^{k,l} = Q_n^{(\alpha+k,\beta+l)}$ with $k, l \in \{0,1\}$, $k+l > 0$. Specifically, we will need the following corollary which comes out of representing $Q_n^{1,0}$ through $Q_n^{0,0}$ [90, equation (3.4)]:

Proposition 2.3.2. Adjacent Jacobi polynomials $Q_n^{1,0}$ are positive definite on Ω.

On the other hand, adjacent polynomials $Q_n^{1,1}$, defined as orthogonal with respect to the measure $(1-t^2)\, d\nu^{(\alpha,\beta)}$, are not positive definite. The following property, a special case of the strengthened Krein condition [91, Lemma 3.22], can serve as a substitute.

Lemma 2.3.3. $(t+1)Q_n^{1,1}(t)$ are positive definite on Ω for $n \geq 0$.

Proof. For all $n \in \mathbb{N}_0$, $(t+1)Q_n^{1,1}$ is orthogonal to all polynomials of degree less than n with respect to the measure $(1-t)d\nu^{(\alpha,\beta)} = c_{\alpha,\beta} d\nu^{(\alpha+1,\beta)}$, so it can be expressed through the orthogonal polynomials corresponding to $d\nu^{(\alpha+1,\beta)}$ as

$$(t+1)Q_n^{1,1}(t) = Q_{n+1}^{1,0}(t) + bQ_n^{1,0}(t),$$

for some constant b. Since all the roots of $Q_n^{1,0}$ lie in $(-1,1)$, $\operatorname{sgn} Q_n^{1,0}(-1) = (-1)^n$. Substituting $t = -1$ in the last equation gives $Q_{n+1}^{1,0}(-1) + bQ_n^{1,0}(-1) = 0$, and so $b \geq 0$. By Proposition 2.3.2, each $Q_n^{1,0}(t)$ is positive definite, and thus $(t+1)Q_n^{1,1}(t)$ is also positive definite. □

Lastly, we will need the strict positive-definiteness of polynomials annihilated by subsets of roots of $p_n + \gamma p_{n-1}$. We recall the following result.

Proposition 2.3.4 ([33, Theorem 3.1])**.** Given a sequence of orthogonal polynomials $p_0(t)$, $p_1(t)$, $p_2(t), \ldots$, let $t_1 < \ldots < t_n$ be the zeros of $p_n + \gamma p_{n-1}$ for some fixed γ. Then the polynomials

$$\prod_{i=1}^{k}(t - t_i), \qquad 1 \leq k < n,$$

can be represented as a linear combination of $p_0(t), p_1(t), \ldots, p_n(t)$ with positive coefficients.

2.3.3 Hermite interpolation

Let $f \in C^K[a, b]$, for some $K \in \mathbb{N}_0$, and let a collection $t_1 < \ldots < t_m \subset [a, b]$, as well as positive integers $k_1, \ldots, k_m$ be given with

$$\max\{k_1, \ldots, k_m\} \leq K + 1.$$

There exists a polynomial p of degree less than $D = \sum_{i=1}^{m} k_i$, such that for $1 \leq i \leq m$ and $0 \leq k < k_i$,

$$p^{(k)}(t_i) = f^{(k)}(t_i).$$

Such a p is called the *Hermite interpolating polynomial* of f; it always exists and is unique because the linear map that takes a polynomial p of degree less than D to

$$(p(t_1), p'(t_1), \ldots, p^{(k_1-1)}(t_1), p(t_2), p'(t_2), \ldots, p^{k_m-1}(t_m))$$

is bijective.

It is convenient to organize both the collection $t_1 < \ldots < t_m$ and the orders of derivatives

$k_1, \ldots, k_m$ into a polynomial $g(t)$. Given such a polynomial

$$g(t) = \prod_{i=1}^{m} (t - t_i)^{k_i},$$

where $D = \deg(g) \geq 1$, we write $H\,[f, g]$ for the interpolating polynomial of degree less than D that agrees with f at each t_i to the order k_i. Similarly, we let

$$Q[f, g](t) = \frac{f(t) - H\,[f, g]\,(t)}{g(t)},$$

be the *divided difference* associated with the polynomial g. Under the above hypotheses, for every $t \in [a, b]$ and a collection $t_1 < t_2 < \ldots < t_m$ as above, there exists $\xi \in (a, b)$ such that $\min(t, t_1) < \xi < \max(t, t_m)$, and

$$Q[f, g](t) = \frac{f^{(D)}(\xi)}{D!}. \tag{2.3.1}$$

Enumerate the roots of g with multiplicities in increasing order, and denote these by $s_j, 1 \leq j \leq D$, where $s_j \leq s_{j+1}$. Let g_n be the polynomial annihilated on the first n elements of the sequence $s_1, \ldots, s_D$:

$$g_n(t) = \prod_{j=1}^{n} (t - s_j), \qquad 1 \leq n \leq D.$$

The usual assignment of the empty product applies here: $g_0(t) = 1$.

By the Newton's formula [43, Chapter 4.6–7], the Hermite interpolating polynomial $H\,[f, g]$ can be represented as

$$H\,[f, g]\,(t) = f(s_1) + \sum_{j=1}^{D-1} g_j(t)\, Q[f, g_j](s_{j+1}). \tag{2.3.2}$$

The relevant property of the p-frame kernel $\left(\frac{s+1}{2}\right)^{p/2}$ considered on a projective space $\mathbb{FP}^{d-1}$, is that its first several derivatives are nonnegative on $(-1, 1)$, followed by a negative one. Positivity of the derivatives implies, due to (2.3.1), that the divided differences in the formula (2.3.2) for the p-frame kernel are nonnegative. It will be convenient to introduce notation for this number of nonnegative derivatives of a function.

Definition 2.3.5. Let $f \in C^M(a,b)$. We say that f is absolutely monotonic of degree M if $f^{(k)}(t) \geq 0$ for $0 \leq k \leq M$ and $t \in (a,b)$.

Compare the above definition with that of absolutely monotonic functions, where all derivatives of a function are non-negative. Usefulness of this pattern of signs of the derivatives lies in that the Hermite interpolant of an absolutely monotonic function f of degree M with $(M+1)$st derivative negative, will stay below f, as shown in the following observation [161].

Lemma 2.3.6. Let $f : [-1,1] \to \mathbb{R}$ be absolutely monotonic of degree M, and $f^{(M+1)}(t) \leq 0$ for all $t \in (-1,1)$. If the roots of a polynomial g of degree $M+1$ are contained in $[-1,1]$, and in addition $g(t) \leq 0$ for $t \in [-1,1]$, then,

$$f(t) \geq H[f,g](t), \qquad t \in [-1,1].$$

Proof. According to (2.3.1), there exists $\xi \in (-1,1)$ such that $\min(t,t_0) < \xi < \max(t,t_M)$, where the roots of g are $t_0 \leq \ldots \leq t_M$, and

$$f(t) - H[f,g](t) = \frac{f^{(M+1)}(\xi)}{(M+1)!} g(t).$$

The expression on the right is nonnegative, so the conclusion of the lemma follows. □

2.3.4 Optimality of tight designs

As above, Ω is a compact, connected two-point homogeneous space and $Q_0, Q_1, Q_2, \ldots$ are the corresponding orthogonal polynomials. Recall that Q_n are orthogonal with respect to the measure $d\nu^{(\alpha,\beta)} = \frac{1}{\gamma_{\alpha,\beta}}(1-t)^\alpha(1+t)^\beta dt$, where the parameters α, β are chosen as in Section 2.2.1. The main result of this section is the following.

Theorem 2.3.7. Let f be absolutely monotonic of degree M, with $f^{(M+1)}(t) \leq 0$ for $t \in (-1, 1)$. Then for a tight M-design $\mathcal{C}$,

$$\mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of

$$I_f(\mu) = \int_\Omega \int_\Omega f(\tau(x, y))\, d\mu(x) d\mu(y)$$

over $\mathcal{P}(\Omega)$, the set of probability measures on Ω.

In what follows we give a proof of the above theorem, splitting it into two separate cases, depending on whether the code $\mathcal{C}$ contains two points separated by the diameter of Ω; equivalently, depending on the parity of the degree M of $\mathcal{C}$.

Proposition 2.3.8. Theorem 2.3.7 holds when $M = 2m$, $m \geq 1$.

Proof. Let $t_1 < \ldots < t_m < t_{m+1} = 1$ be the values of $\tau(x, y) = \cos(\vartheta(x, y))$ occurring in $\mathcal{C}$. Let further

$$g_k(t) = \prod_{i=1}^{k} (t - t_i), \qquad 1 \leq k \leq m + 1.$$

and

$$g(t) = g_m(t)\, g_{m+1}(t) = (t - 1) g_m^2(t).$$

To prove the statement of the theorem, we verify the following chain of inequalities, satisfied for arbitrary $\mu \in \mathcal{P}(\Omega)$, similar to the proof of Lemma 2.3.1,

$$I_f(\mu) \geq I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma) = I_{H[f,g]}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}). \tag{2.3.3}$$

The equality $I_{H[f,g]}(\sigma) = I_{H[f,g]}(\mu_{\mathcal{C}})$ follows since $\mathcal{C}$ is a design of degree $2m \geq \deg H[f, g]$. The last equality holds since $H[f, g]$ agrees with f at the cosines of distances occurring in $\mathcal{C}$. Since $g(t) \leq 0$ for $t \in [-1, 1]$, Lemma 2.3.6 implies that $f(t) \geq H[f, g](t)$, $t \in [-1, 1]$, which gives the first inequality. It remains to show the second inequality: it will follow from the positive definiteness of $H[f, g]$, which we will now demonstrate.

For any $n < m$, the degree of $g_{m+1}(t)Q_n(t)$ is at most $2m$. As $\mathcal{C}$ is a $2m$-design, for every fixed $y \in \mathcal{C}$ there holds

$$\begin{aligned}\int_{-1}^{1} g_{m+1}(t)Q_n(t)d\nu^{(\alpha,\beta)} &= \int_{\Omega} g_{m+1}(\tau(x,y))Q_n(\tau(x,y))d\sigma(x) \\ &= \frac{1}{|\mathcal{C}|}\sum_{x\in\mathcal{C}} g_{m+1}(\tau(x,y))Q_n(\tau(x,y)) \\ &= \frac{1}{|\mathcal{C}|}\sum_{i=1}^{m+1} c_i g_{m+1}(t_i)Q_n(t_i) \\ &= 0,\end{aligned}$$

since, by construction, g_{m+1} is annihilated on all the t_i. The constants c_i are given by

$$c_i = |\{x \in \mathcal{C} \mid \tau(x,y) = t_i\}|.$$

Both g_{m+1} and Q_{m+1} are monic, so we conclude that

$$g_{m+1}(t) = Q_{m+1}(t) + \gamma Q_m(t),$$

for some $\gamma \in \mathbb{R}$. By Proposition 2.3.4, subproducts of zeros of g_{m+1}, which we denote by g_k, $1 \leq k \leq m$, can be expressed as linear combinations of Q_n with positive coefficients, and therefore are positive definite.

According to the Newton's formula (2.3.2), the Hermite interpolant of f can be expressed as the sum of partial products of factors of g multiplied by the appropriate divided difference. We will use this formula to show that $H[f,g]$ is positive definite. Indeed, (2.3.2) gives

$$H\left[f,g\right](t) = f(t_1) + \sum_{k=1}^{m}\left(g_k(t)g_{k-1}(t)\,Q\left[f, g_k g_{k-1}\right](t_k) + g_k^2(t)\,Q\left[f, g_k^2\right](t_{k+1})\right),$$

where as usual, $g_0 = 1$. Observe that the divided differences in the last equation are nonnegative due to (2.3.1), as the function f is absolutely monotonic of degree $2m$. Since we have shown that each g_k is positive definite, Schur's theorem implies that so are g_k^2 and $g_k g_{k+1}$, and it follows that $H[f,g]$ is positive definite as well.

$\square$

Before turning to the proof of Theorem 2.3.7 for tight designs of odd strength, recall the definition of the adjacent polynomials $Q_n^{1,1} = Q_n^{(\alpha+1,\beta+1)}$ for $n \geq 0$. They are monic, orthogonal with respect to the measure

$$d\nu^{(\alpha+1,\beta+1)}(t) = \frac{1}{\gamma_{\alpha+1,\beta+1}}(1-t)^{\alpha+1}(1+t)^{\beta+1}dt = \frac{\gamma_{\alpha,\beta}}{\gamma_{\alpha+1,\beta+1}}(1-t^2)d\nu^{(\alpha,\beta)}(t),$$

since the polynomials $Q_n^{(\alpha,\beta)}(t)$ are orthogonal with respect to measure $d\nu^{(\alpha,\beta)}$.

Proposition 2.3.9. Theorem 2.3.7 holds when $M = 2m-1$, $m \geq 1$.

Proof. Suppose that $\mathcal{C} \subset \Omega$ is a tight $(2m-1)$-design. As discussed in Section 2.2.3 tight designs of odd strength necessarily contain antipodal points, i.e. there exist $x, y \in \mathcal{C}$ such that $\vartheta(x,y) = \pi$ and thus $-1 \in \mathcal{A}(\mathcal{C}) = \{\tau(x,y) | \, x, y \in \mathcal{C}\}$. Let $-1 = t_1 < \ldots < t_m < t_{m+1} = 1$ be the values of $\tau(\vartheta(x,y))$ for $x, y \in \mathcal{C}$. Let further

$$w(t) = \prod_{j=2}^{m}(t - t_j)$$

and

$$g(t) = w^2(t)(t^2-1).$$

As in the proof of Proposition 2.3.8, we need to verify the inequalities (2.3.3). Applying Lemma 2.3.6 to $H[f,g]$ gives the first inequality; it remains to show positive-definiteness of $H[f,g]$.

For $n < m-1$, the degree of $(1-t^2)w(t)Q_n^{1,1}(t)$ is at most $2m-1$, so for any $y \in \mathcal{C}$ there holds

$$
\begin{aligned}
\frac{\gamma_{\alpha+1,\beta+1}}{\gamma_{\alpha,\beta}} \int_{-1}^{1} w(t) Q_n^{1,1}(t) d\nu^{(\alpha+1,\beta+1)} &= \int_{\Omega} (1-\tau^2(x,y)) w(\tau(x,y)) Q_n^{1,1}(\tau(x,y)) d\sigma(x) \\
&= \frac{1}{|\mathcal{C}|} \sum_{x\in\mathcal{C}} (1-\tau^2(x,y)) w(\tau(x,y)) Q_n^{1,1}(\tau(x,y)) \\
&= \frac{1}{|\mathcal{C}|} \sum_{j=1}^{m+1} c_j (1-t_j^2) w(t_j) Q_n^{1,1}(t_j) \\
&= 0,
\end{aligned}
$$

as $(1-t^2)w(t)$ is annihilated on the cosines of distances from $\mathcal{C}$. Because $w(t)$ is a degree $m-1$ monic polynomial, the above implies $w(t) = Q_{m-1}^{1,1}(t)$. By Proposition 2.3.4, this also means that for $2 \le k \le m-1$, polynomials $\prod_{j=2}^{k}(t-t_j)$ are linear combinations of $Q_n^{1,1}$ with nonnegative coefficients. Since the cone of functions with nonnegative Jacobi coefficients with respect to $Q_n^{1,1}$ is closed under multiplication, polynomials $\prod_{j=2}^{k}(t-t_j)^2$ and $(t-t_k)\prod_{j=2}^{k-1}(t-t_j)^2$ also have nonnegative Jacobi coefficients in $Q_n^{1,1}$. Due to Lemma 2.3.3, since $t - t_1 = t+1$, we obtain that

$$
a_k(t) := (t-t_1)(t-t_l) \prod_{j=2}^{k-1} (t-t_j)^2 \quad \text{and} \quad b_k(t) := (t-t_1) \prod_{j=2}^{k} (t-t_j)^2, \tag{2.3.4}
$$

are linear combinations of $Q_n^{(\alpha,\beta)}$ with positive coefficients, that is, they are positive definite on Ω for $1 \le k \le m$.

We conclude by the same observations as in the proof of Proposition 2.3.8; in particular, the positive definiteness of the Hermite interpolant $H[f,g]$ follows from the representation

$$
H\left[f,g\right](t) = f(t_1) + \sum_{k=2}^{m-1} \Big(a_k(t)\, Q\left[f, a_k\right](t_k) + b_k(t)\, Q\left[f, b_k\right](t_{k+1}) \Big),
$$

combined with the absolute monotonicity of f to degree $2m-1$, which implies positivity of the divided differences Q. □

Example 2.3.10. As an example of another application of Theorem 2.3.7, consider the case that

$f(t) = a + bt + ct^2 + dt^3$ is given as potential function. By the results in Chapter 1 we know already that there is a discrete minimizer for any energy with a polynomial potential function as above. In this case, some elementary considerations show that if

(i) $d \le 0$,

(ii) $c \ge -3d$,

(iii) $c^2 - 3bd \ge 0$,

(iv) $-c - \sqrt{c^2 - 3bd} \le 3d$, and,

(v) $-c + \sqrt{c^2 - 3bd} \ge 3d$,

then f is absolutely monotonic of degree 2 up to a constant. Hence, any potential function of the above form has as minimizer of the f-energy on any of the projective spaces a tight 2-design. In particular, for f as above, the icosahedron is a minimizer of energy integral $I_f(\mu)$ over symmetric measures on the sphere $\mathbb{S}^2$. Note that the constant term can be ignored, so it suffices to only consider the sign of derivatives. In particular, if $b > 0$ and d becomes sufficiently small in magnitude, the above inequalities will hold.

For comparison, on $\mathbb{S}^2$, $f(\tau(x, y)) = f(2|\langle x, y\rangle|^2 - 1)$ is positive definite (up to a constant), precisely when $\widehat{f}_1$, $\widehat{f}_2$, and $\widehat{f}_3$ are positive, or equivalently (by calculation),

(i) $4b - 2c + 3d \ge 0$,

(ii) $2c - d \ge 0$, and,

(iii) $d \ge 0$.

Thus, I_f is minimized by the surface measure σ precisely for the coefficients satisfying the above inequalities.

2.3.5 Uniqueness of minimizers supported on tight designs

The proofs in the last section left the question of uniqueness of minimizers open. Are there any other minimizers for p-frame energies when tight designs minimize and p is not an even integer? The answer, as this section details, is no.

Whenever a tight design minimizes I_f, any minimizer for an energy with kernel f that is absolutely monotonic to degree M, and which satisfies $f^{(M+1)}(t) < 0$, $t \in (-1, 1)$, is minimized only on a tight design, although such designs are not necessarily unique up to equivalence (see Section 2.9 for more details).

To prove uniqueness, up to tightness, we consider the spherical and projective cases separately, although within the same general framework. Let $\mathcal{C}$ be a finite m-distance set in $\Omega = \mathbb{S}^{d-1}$ or $\mathbb{FP}^{d-1}$ with $\mathcal{A}(\mathcal{C}) = \{\tau(x, y) \mid x, y \in \mathcal{C}\}$, so that $m = |\mathcal{A}(\mathcal{C})| - 1$. Set $e = |\mathcal{A}(\mathcal{C}) \setminus \{-1\}| - 1$ and ϵ to be 1 if $-1 \in \mathcal{A}(\mathcal{C})$ and 0 otherwise, i.e. $e = m - \epsilon$. The annihilating polynomial of a configuration $Ann(\mathcal{C})$ is defined by $\Pi_{\alpha \in \mathcal{A}(\mathcal{C})}(x - \alpha)$. For a positive number t, let $(t)_k = t(t+1)\ldots(t+k-1)$ be the Pochhammer symbol, and let $\mathcal{T}$ be a tight design of size N in Ω. The following lemmas from [44] and [73] provide some additional properties of tight designs which will be useful in the theorem which follows.

Lemma 2.3.11. Let $\mathcal{C}$ be an m-distance configuration, $\mathcal{C} \subset \mathbb{S}^{d-1}$, $|\mathcal{C}| = N$

(i) If $\mathcal{C}$ is a t-design, then $t \leq 2m$ and $N \leq \binom{d+m-1}{d-1} + \binom{d+m-2}{d-1}$. Equality holds in either of these inequalities if and only if $\mathcal{C}$ is a tight $2m$-design and $Ann(\mathcal{C}) = Ann(\mathcal{T})$.

(ii) If $\mathcal{C}$ is an antipodal t-design, then $t \leq 2m - 1$, and $N \leq \binom{d+m-2}{d-1}$. Equality holds in either of these inequalities if and only if $\mathcal{C}$ is a tight $(2m-1)$-design, and in particular $Ann(\mathcal{C}) = Ann(\mathcal{T})$.

The projective analog of the above lemma is now given.

Lemma 2.3.12. For an m-distance configuration $\mathcal{C} \subset \mathbb{FP}^{d-1}$, $|\mathcal{C}| = N$,

(i)

$$N \leq \frac{(\alpha+1)_m(\alpha+1-\beta)_\epsilon}{(\beta+1)_m e!}$$

and equality holds if and only if $\mathcal{C}$ is a tight $(2m-1)$-design and $Ann(\mathcal{C}) = Ann(\mathcal{T})$.

(ii) If $\mathcal{C}$ is a t-design but not a $(t+1)$-design, then $t \leq m+e$ with equality if and only if equality holds in part one of this lemma.

The annihilating polynomials for tight designs can be worked out explicitly and are given in [73]. We now show uniqueness of minimizing measures in Theorem 2.3.7.

Theorem 2.3.13. Suppose that a tight M-design $\mathcal{C}$ minimizes the f-energy integral, for f absolutely monotonic of degree M and such that $f^{(M+1)}(t) < 0$, $t \in (-1,1)$. Then any minimizer of $I_f(\mu)$ must be a tight M-design.

Proof. The argument developed to prove Theorem 2.3.7 may be described concisely through the following string of inequalities

$$I_f(\mu) \geq I_h(\mu) \geq I_h(\sigma) = I_h(\nu) = I_f(\nu).$$

In order for $I_f(\mu) = I_f(\nu)$ to hold, the first inequalities must be equalities. The first inequality can only be sharp in the case that the values $\tau(x,y)$, $x, y \in \operatorname{supp}\mu$ are a subset of those given for $x, y \in \operatorname{supp}\xi$, where ξ is the minimizing tight design. This follows from the fact that $h(t) < f(t)$ for all t outside this set by the remainder formula from Lemma 2.3.6. In particular, this gives that $|\operatorname{supp}\mu|$ is finite.

The second inequality is sharp only when μ is a weighted design of at least the order corresponding to the minimizing tight design. By the above lemma μ then satisfies $\mathcal{A}(\operatorname{supp}\mu) \subset \mathcal{A}(\operatorname{supp}\xi)$. Since tight designs maximize the size of a code over all m-distance sets, where $m = |\mathcal{A}(\operatorname{supp}\xi)|$, finally it holds that $|\mathcal{A}(\operatorname{supp}\mu)| = |\mathcal{A}(\operatorname{supp}\xi)|$ and $|\operatorname{supp}\mu| = |\operatorname{supp}\xi|$, so that μ must be tight. □

2.4 Optimality of the 600-cell

This section concerns only the p-frame kernels; it will be shown here that the 600-cell minimizes the p-frame energy on $\mathbb{S}^3$ for a certain range of p. The 600-cell is one of the six 4-dimensional convex regular polytopes; it has 600 tetrahedral faces, which explains the origin of its name. When its 120 vertices are identified with unit quaternions, they give a representation of the elements of a group known as the binary icosahedral group [137].

As discussed above (2.2.4), optimization of p-frame energy on the sphere $\mathbb{S}^3$ is equivalent to optimization of the expression $\iint_{(\mathbb{RP}^3)^2} f(\tau(x,y))\,d\mu(x)d\mu(u)$ over measures μ on $\mathbb{RP}^3$, where the kernel f is given by

$$f(t) = \left(\frac{1+t}{2}\right)^{\frac{p}{2}}.$$

We therefore assume for the rest of this section the underlying space to be $\mathbb{RP}^3$, and use the corresponding Jacobi polynomials $C_n^{(-1/2,1/2)}(t)$. Following the approach of the previous section, we will establish a sequence of inequalities similar to (2.3.3).

The 600-cell is only a projective 5-design and therefore not tight, cf. Table A.1. The authors in [33], motivated by an approach found in the paper [2], found means to prove universal optimality of the 600-cell by using a higher degree interpolating polynomial. The 600-cell has the notable property that 7th, 8th, and 9th degree harmonic averages over it vanish, although the 6th degree average does not. This allows for constructing a degree 8 polynomial h which is less than or equal to f, positive definite, and agrees with f at the distances appearing in the 600-cell, and which finally has the property that its 6th Jacobi coefficient vanishes.

For a polynomial h of the form,

$$h = \sum_{\substack{n=0 \\ n\neq 6}}^{8} \widehat{h}_n\, C_n^{(1/2,-1/2)}(t), \tag{2.4.1}$$

the coefficients $\widehat{h}_n$ can be uniquely determined as functions of p by setting

$$\begin{aligned} h(t_i) =& f(t_i), \qquad 1 \le i \le 5 \\ h'(t_i) =& f'(t_i), \qquad 2 \le i \le 4, \end{aligned}$$

where $-1 = t_1 < t_2 < \ldots < t_5 = 1$ are the values of $\tau(x, y)$ when vectors x, y vary over the vertices of the 600-cell, see the proof of Theorem 2.4.2 below and Table A.1. It turns out that for all $p \in [8, 10]$, $\widehat{h}_n(p) \ge 0$ when $0 \le n \le 8, n \ne 6$. We apply a computer-assisted approach to verify this positivity; specifically, using interval arithmetic, we compute values of $\widehat{h}_n(p)$ on a grid fine enough to guarantee that $\widehat{h}_n(p) \ge 0$. The details of this computation are available in the appendix, see Section A.2. Even though the computations performed are carried out in finite floating point precision, interval arithmetic guarantees that the results of these computations lie in precisely defined intervals (using libraries [108, 164, 126]). The computer-assisted argument yields the following.

Lemma 2.4.1. If $p \in [8, 10]$ and the polynomial h is constructed as above, the coefficients $\widehat{h}_n$ in the Jacobi expansion (2.4.1) satisfy $\widehat{h}_n(p) \ge 0$.

Using this fact we show optimality of the 600-cell on the range $p \in [8, 10]$.

Theorem 2.4.2. The 600-cell minimizes the p-frame energy for $p \in [8, 10]$ over Borel probability measures on $\mathbb{S}^3$ or $\mathbb{RP}^3$.

Proof. Let $f(t) = \left(\frac{t+1}{2}\right)^{p/2}$ for some $8 < p < 10$, $t_1 = -1$, $t_2 = \frac{-\sqrt{5}-1}{4}$, $t_3 = -\frac{1}{2}$, $t_4 = \frac{\sqrt{5}-1}{4}$, and $t_5 = 1$. Let $h(t)$ be the 8th degree polynomial given by (2.4.1), such that $h(t_i) = p(t_i)$ for $1 \le i \le 5$, and $h'(t_i) = p'(t_i)$ for $2 \le i \le 4$. By Lemma 2.4.1, the coefficients $\widehat{h}_n$ are non-negative for $p \in [8, 10]$.

Let $p(t) = (t^2 - 1) \prod_{i=2}^{4} (t - t_i)^2$ and $\tilde{h}(t) = H[f, p](t)$. Then we also have $\tilde{h}(t) = H[h, p](t)$. This gives

$$f(t) - \tilde{h}(t) = \frac{f^{(8)}(\xi)}{8!} p(t) \ge 0,$$

and

$$h(t)-\tilde{h}(t)=\frac{h^{(8)}(\nu)}{8!}p(t)\leq 0.$$

We thus have $f(t)-h(t)=f(t)-\tilde{h}(t)+\tilde{h}(t)-h(t)\geq 0$. Since $h(t)$ is positive definite and $\widehat{h}_6=0$, for the 600-cell $\mathcal{C}_{600}$, we have the following sequence of inequalities

$$I_f(\mu)\geq I_h(\mu)\geq I_h(\sigma)=I_h(\mu_{\mathcal{C}_{600}})=I_f(\mu_{\mathcal{C}_{600}}),$$

implying that equally weighted vertices of $\mathcal{C}_{600}$ minimize p-frame energy. □

2.5 Conjectured minimizers

2.5.1 New small weighted projective design

We now collect facts on the 85 vector system which was found while numerically minimizing the $p=5$ frame potential in $\mathbb{C}^5$. This system of vectors forms a weighted design of strength 3, or equivalently, for the functional $\sum_{i,j}|\langle v_i,v_j\rangle|^6\omega_i\omega_j$, the weighted system takes the value $1/35$, thus minimizing this quantity over all probability measures $\mu=\sum_i\delta_{v_i}\omega_i$, $\sum_i\omega_i=1$ supported on unit vectors $\|v_i\|=1$ in $\mathbb{C}^5$ [154]. The above construction appears to be new especially when comparing its size to previously obtained bounds from [96] for smallest known 3 weighted designs in $\mathbb{C}^5$.

One part of the system is well studied, given by the root vectors corresponding to the 45 2-reflections which generate the unitary reflection group $W(K_5)$ of 51840 elements [87]. This group is alternatively described as the group $G_3(10)\simeq(C_6\times SU_4(2)):C_2$, one of the maximal finite irreducible subgroups of $GL_{10}(\mathbb{Z})$ [136]. $SU_4(2)$ here is just the special linear group of 4×4 matrices, unitary matrices over $\mathbb{F}_{2^2}$, with determinant one.

Choosing the representation of the root vectors in $W(K_5)$ as $X_1=\{\sigma((1,0,0,0,0))\}\cup\{\sigma(\frac{1}{2}(0,1,\pm\omega,\pm\omega,\pm 1))\}$ under cyclic coordinate permutations, σ, the new weighted design arises when this system is joined with some other 40 vectors. The second system may be described as $\Psi=\{\sigma(\frac{1}{\sqrt{3}}(1,0,\pm\omega,\pm\omega,0))\}\cup\{\sigma(\frac{1}{\sqrt{3}}(1,\pm\omega,\pm 1,0,0))\}$ also generated under cyclic coordinate permutations. The projective design is finally given by assigning weights to the $W(K_5)$ system joined with the 40 vector system after giving Ψ the orientation $X_2 = U\Psi$, where

$$U = \frac{1}{2}\begin{bmatrix} 1 & -\omega & -\omega & 1 & 0 \\ -1 & 1 & -\omega^2 & 0 & -\omega^2 \\ \omega^2 & 0 & -\omega^2 & 1 & 1 \\ 0 & 1 & \omega & -\omega & -1 \\ \omega^2 & \omega & 0 & -\omega & \omega^2 \end{bmatrix}, \tag{2.5.1}$$

is unitary ($\omega = e^{2\pi i/3}$). With the above orientation the 40 points in X_2 appear to fit so that each point is a maximizer of the projective distance from each of the 45 vectors in the $W(K_5)$ system and vice versa. If so, the additional 40 points satisfy that they are the points at greatest distance from the original 45, in particular.

To form a weighted 3-design, the corresponding weights for X_1, the 45 vector system, are $\omega_1 = \frac{4}{315}$, and for the remaining 40 vectors in X_2, the weights are $\omega_2 = \frac{3}{280}$. In total the distribution of absolute values of inner products that appears in the unweighted 85 vector system is given in Table 2.5. The supplementary files in the arXiv version of this manuscript provide a magma script which verifies that $\sum_{i,j}|\langle v_i, v_j\rangle|^6\omega_i\omega_j = 1/35$, so that the system is a projective 3-design. This script can additionally be used to show the automorphism group of the above system of 85 vectors is isomorphic to the group $SU_4(2)$ of order $|SU_4(2)|= 25920 = 2^6 \cdot (2^4 - 1) \cdot (2^3 + 1) \cdot (2^2 - 1)$, through use of a library from [74].

The above construction hides the relation between its two parts. The 85 vectors in $\mathbb{C}^5$ may be seen, after canonically embedding the vectors in $\mathbb{R}^{10}$, as the weighted union of vectors coming from two 10 dimensional lattices. Under this identification, the 45 vectors in the $W(K_5)$ system may be selected as, up to projective equivalence (modulo multiples of sixth roots of unity), the 270 minimal vectors of the lattice called $(C_6 \times SU_4(2)) : C_2$ in the database [110], and the other 40 points are taken one from each antipodal pair of the 80 minimal vectors of the shorter Coxeter-Todd lattice, O_{10} detailed in [118]. The relationship between these two lattices is that $(C_6 \times SU_4(2)) : C_2$ is similar to the maximal even sub-lattice of O_{10}. In our tables, we choose to name these the $W(K_5)$ and O_{10} lattices. We prefer an alternative name for the first since the automorphism group of each lattice is $(C_6 \times SU_4(2)) : C_2$.

Altogether, upon splitting the weights across minimal vectors in appropriately scaled and oriented copies of these lattices and then complexifying everything, one arrives at the cubature formula, which when viewed projectively, is a system of 85 vectors improving on the best previous known bound of size 320 for such a formula (see [132]). Some experiments suggest this might be the smallest sized weighted projective 3-design in $\mathbb{CP}^4$. Expecting that this code might be optimal in a few other settings, we conjecture:

Conjecture 2.5.1. The code constructed in this section of 85 points in $\mathbb{C}^5$ is universally optimal.

This is an example of one of the 'highly symmetric tight frames', as was later demonstrated in [107].

2.5.2 Other weighted designs

11 *points in* $\mathbb{R}^3$

It seems that as p goes to 6 from below, the limiting minimizing configuration on the sphere $\mathbb{S}^2$ is of the following form. Concisely, the system consists of all combinations of signs of the 6 vectors below,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \frac{2}{\sqrt{7}} & \sqrt{\frac{3}{7}} & 0 \\ \frac{2}{\sqrt{7}} & 0 & \sqrt{\frac{3}{7}} \\ \sqrt{\frac{1}{7}} & \sqrt{\frac{3}{7}} & \sqrt{\frac{3}{7}} \end{bmatrix}$$

with the weights,

$$\frac{2}{27}, \frac{1}{10}, \frac{1}{10}, \frac{49}{540}, \frac{49}{540}, \frac{49}{540}$$

on each line. The off-diagonal inner products are then

$$1/7, -1/7, 5/7, -5/7, \sqrt{3/7}, -\sqrt{3/7}, 0, \sqrt{1/7}, -\sqrt{1/7}, 4/7, -4/7, \sqrt{4/7}, -\sqrt{4/7}$$

appearing in number, $(10, 18, 10, 10, 14, 10, 14, 6, 2, 4, 4, 6, 2)$ respectively. From these facts, one may check that the 11 lines defined by these vectors forms a projective 3-design. Notably, this is the same extremal code, which forms a minimal cubature formula and is found also in [120, page 135].

16 *points in* $\mathbb{R}^3$

Lines through antipodal points in the union of a regular icosahedron with its dual dodecahedron. The frequencies of absolute values of inner products are $N(\sqrt{\frac{1}{15}(5-2\sqrt{5})}) = 60$, $N(\frac{\sqrt{75+30\sqrt{5}}}{15}) = 60$, $N(\frac{1}{3}) = 60$, $N(\frac{1}{\sqrt{5}}) = 30$, $N(\sqrt{\frac{5}{9}}) = 30$, and $N(1) = 60$. The weights making this configuration a projective 4-design are $\omega_1 = 5/84$ and $\omega_2 = 9/140$ for the icosahedron and dodecahedron vertices respectively.

11 *points in* $\mathbb{R}^4$

See Table 2.6 for what appears to be the limiting minimizing configuration as p goes to 6 from below when minimizing over $\mathbb{S}^3$.

24 *points in* $\mathbb{R}^4$

The regular 24 cell, or alternatively the D_4 root system. The frequencies of absolute values of inner products are $N(0) = 216,\ N(\frac{1}{\sqrt{2}}) = 144,\ N(\frac{1}{2}) = 192,$ and $N(1) = 24.$ The configuration is unweighted as a projective 3-design.

16 *points in* $\mathbb{R}^5$

Lines through antipodal points in the following construction. Take all permutations of $\pm\frac{1}{\sqrt{30}}(-5,1,1,1,1,1,1)$ and $\frac{1}{\sqrt{6}}(1,1,1,-1,-1,-1)$ and consider these as vectors in the copy of $\mathbb{S}^4$ in $\mathbb{S}^5$ on the plane perpendicular to $(1,1,1,1,1,1)$. The frequencies of absolute values of inner products are $N(\frac{1}{3})=90,\ N(\frac{1}{5})=30,\ N(\frac{1}{\sqrt{5}})=120,$ and $N(1)=16$. The weights making this a projective 2-design are $\omega_1=\frac{5}{84}$ and $\omega_2=\frac{9}{140}$ for the above parts respectively.

41 *points in* $\mathbb{R}^5$

An example of a design construction appearing in [139]. The configuration comprises of lines through antipodal points in the following construction. Let A be the set of vectors which are permutations of $(\pm1,0,0,0,0)$, B permutations of $(\pm\sqrt{\frac{1}{2}},\pm\sqrt{\frac{1}{2}},0,0,0)$, and C permutations of $(\pm\sqrt{\frac{1}{5}},\pm\sqrt{\frac{1}{5}},\pm\sqrt{\frac{1}{5}},\pm\sqrt{\frac{1}{5}},\pm\sqrt{\frac{1}{5}})$. The frequencies of absolute values of inner products are $N(0)=600,\ N(\frac{1}{5})=160,\ N(\frac{3}{5})=80,\ N(\sqrt{\frac{1}{5}},\ N(\sqrt{\frac{2}{5}})=320,$ and $N(1)=41$. The weights making this a projective 3-design are $\omega_1=\frac{2}{105}$, $\omega_2=\frac{8}{315}$, and $\omega_3=\frac{25}{1008}$, on $A,B,$ and C respectively.

22 *points in* $\mathbb{R}^6$

Lines through antipodal points in a hemicube/cross polytope compound, where the hemicube is within the cube dual to the cross polytope. The frequencies of absolute values of inner products are $N(0)=30,\ N(\frac{1}{\sqrt{6}})=192,\ N(\frac{1}{3})=240,$ and $N(1)=22$. The weights making this a projective 2-design are $\omega_1=3/64$ on the hemicube and $\omega_2=1/24$ on the cross-polytope.

63 *points in* $\mathbb{R}^6$

Lines through antipodal points in the union of minimal vectors of E_6 and its dual lattice, E_6^*. The frequencies of absolute values of inner products are $N(0)=1620,\ N(\frac{1}{4})=432,\ N(\frac{1}{2})=990,\ N(\sqrt{\frac{3}{8}})=864,$ and $N(1)=63$. The weights making this a projective 3-design are $\omega_1=1/60$ and $\omega_2=2/135$ on the minimal vectors of E_6 and its dual, respectively.

91 *points in* $\mathbb{R}^7$

The configuration is projectively composed of the union of the minimal vectors of E_7 and its dual lattice, E_7^*. The frequencies of absolute values of inner products are $N(0) = 3906$, $N(\frac{1}{27}) = 756$, $N(\frac{1}{8}) = 2016$, $N(\frac{\sqrt{3}}{9}) = 1512$, and $N(1) = 91$. The weights making this a projective 3-design are $\omega_1 = 8/693$ and $\omega_2 = 3/308$ on the E_7 part and its dual, respectively. The cubature formula appears also in [113].

36 *points in* $\mathbb{R}^8$

The edge midpoints of a regular simplex. The frequencies of absolute values of inner products are $N(\frac{2}{7}) = 756$, $N(\frac{5}{14}) = 504$, and $N(1) = 36$. This code is a projective 1-design with equal weights.

21 *points in* $\mathbb{C}^3$

A structured union of a maximal (tight) simplex (equiangular tight frame, or ETF) of 9 vectors and 4 mutually unbiased bases (a 4-MUB) of 12 vectors. The frequencies of absolute values of inner products are $N(0) = 96$, $N(\frac{1}{2}) = 72$, $N(\frac{1}{\sqrt{3}}) = 108$, $N(\frac{1}{\sqrt{2}}) = 144$, $N(1) = 21$. The weights making this a projective 3-design are $\omega_1 = 4/90$ on the 9-ETF and $\omega_2 = \frac{1}{20}$ on the 4-MUB.

2.6 Energies in non-compact spaces

In the previous sections, we used linear programs to bound energies on compact two-point homogeneous spaces. This approach can be extended to p-frame energies in non-compact spaces as well. Just as above, we consider $\mathbb{F} = \mathbb{R}, \mathbb{C}$, or $\mathbb{H}$. In this setting, we consider the set of probability measures $\mathcal{P}(\mathbb{F}^d)$ with the additional restriction

$$\int_{\mathbb{F}^d} |x|^2 d\mu(x) = 1 \tag{2.6.1}$$

for each $\mu \in \mathcal{P}(\mathbb{F}^d)$. This normalization allows us to obtain a direct extension of above results for the spherical case, and by scaling, solutions to more general problems can be obtained from these results. A similar problem of finding maximizers for p-frame energies for $p \leq 2$, subject to the condition that measures be isotropic, was investigated in [63].

For a potential function $f = f(\tau(x,y))$ we define the energy with respect to measure $\mu \in \mathcal{P}(\mathbb{F}^d)$:

$$I_f(\mu) = \int_{\mathbb{F}^d} \int_{\mathbb{F}^d} f(\tau(x,y)) d\mu(x) d\mu(y).$$

We will be concerned in this section only with the case that $f(\tau(x,y)) = |\langle x, y\rangle|^p$. The Jacobi polynomials for the projective spaces $\mathbb{FP}^{d-1}$, as above, are denoted C_m.

Lemma 2.6.1. For $p \geq 2$, assume $f(t) = \left(\frac{t+1}{2}\right)^{\frac{p}{2}} \geq h(t) = \sum\limits_{m=0}^{\infty} \widehat{h}_m C_m(t)$ for all $t \in [-1,1]$, where $\widehat{h}_m \geq 0$ for all $m \geq 0$. Then $I_f(\mu) \geq \widehat{h}_0$ for all $\mu \in \mathcal{P}(\mathbb{F}^d)$ satisfying (2.6.1).

Proof. Since discrete masses are weak-$*$ dense in $\mathcal{P}(\mathbb{F}^d)$, it is sufficient to prove the inequality for them only. Let μ take the form $\mu = \frac{1}{N}\sum\limits_{i=1}^{N} \delta_{x_i}$, $x_i \in \mathbb{F}^d$ and set $y_i = \frac{x_i}{|x_i|}$. Then,

$$I_f(\mu) = \frac{1}{N^2}\sum_{i,j=1}^{N} |\langle x_i, x_j\rangle|^p = \frac{1}{N^2}\sum_{i,j=1}^{N} |x_i|^p |x_j|^p |\langle y_i, y_j\rangle|^p$$

$$\geq \frac{1}{N^2}\sum_{i,j=1}^{N} |x_i|^p |x_j|^p h(\tau(y_i,y_j)) = \frac{1}{N^2}\sum_{m=0}^{\infty} \widehat{h}_m \sum_{i,j=1}^{N} |x_i|^p |x_j|^p C_m(\tau(y_i,y_j)).$$

For any $m \geq 1$, C_m is positive definite on $\mathbb{FP}^{d-1}$ so that each sum $\sum\limits_{i,j=1}^{N} |x_i|^p |x_j|^p C_m(\tau(y_i,y_j))$ is non-negative. Thus,

$$I_f(\mu) \geq \widehat{h}_0 \frac{1}{N^2}\sum_{i,j=1}^{N} |x_i|^p |x_j|^p C_0(\tau(y_i,y_j)) = \widehat{h}_0 \left(\frac{1}{N}\sum_{i=1}^{N} |x_i|^p\right)^2.$$

Since $p \geq 2$,

$$\frac{1}{N}\sum_{i=1}^{N} |x_i|^p \geq \left(\frac{1}{N}\sum_{i=1}^{N} |x_i|^2\right)^{\frac{p}{2}},$$

holds by Jensen's inequality. The constraint 2.6.1 is equivalent to $\frac{1}{N}\sum_{i=1}^{N}|x_i|^2=1$, and so combining all inequalities, we complete the proof of the lemma. $\square$

Lemma 2.6.1 gives that any linear programming bounds for p-frame energies applicable to the spherical/projective case will work in the non-compact setting as well. As a consequence of this approach we obtain the following result.

Theorem 2.6.2. Let $\mathcal{C}$ be a set of arbitrary unit representatives of a tight projective M-design, $M \geq 2$, in $\mathbb{FP}^{d-1}$ and $f(\tau(x,y)) = |\langle x, y\rangle|^p$ with $p \in [2M-2, 2M]$. Then

$$\mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|}\sum_{x\in\mathcal{C}}\delta_x$$

is a minimizer of

$$I_f(\mu) = \int_{\mathbb{F}^d}\int_{\mathbb{F}^d} f(\tau(x,y))d\mu(x)d\mu(y)$$

over $\mathcal{P}(\mathbb{F}^d)$, the set of probability measures on $\mathbb{F}^d$ satisfying the constraint 2.6.1.

Proof. For the proof, we take $f(t) = \left(\frac{t+1}{2}\right)^{\frac{p}{2}}$ and the interpolating polynomials $H[f,g]$ used in the proof of Theorem 2.3.7 and follow the same line of reasoning there:

$$I_f(\mu) \geq I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma_d) = I_{H[f,g]}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}). \tag{2.6.2}$$

All inequalities are verified in a similar manner as in the previous section, except for $I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma_d)$. This part follows from Lemma 2.6.1 applied to $h = H[f,g]$ because $I_h(\sigma_d)$ is precisely $\widehat{h}_0$ for positive definite functions h. $\square$

To conclude the section, we note that the results analogous to Theorem 2.4.2 on the optimality of the 600-cell and the numerical linear programming bounds for p-frame energies in the compact setting apply to the non-compact setting also.

2.7 Mixed volume inequalities

In this section we demonstrate an intriguing connection between the p-frame energy and convex geometry. We begin by briefly recalling some of the basic notions from convex geometry. See [79, Ch. 2] for a more thorough development.

Let K be a convex body and $\sigma_K(u)$ be the surface measure of K, that is, a measure supported on the unit sphere $\mathbb{S}^{d-1}$, satisfying

$$\sigma_K(B) = |x \in \partial K,\ \text{the outer unit normal to } K \text{ at } x \text{ belongs to } B|_{d-1}$$

for all Borel sets $B \subset \mathbb{S}^{d-1}$, where $|\cdot|_{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure. For example, if K is a polytope with faces $\{K_i\}_{i=1}^m$ and normals $\{n_i\}_{i=1}^m$, σ_K is atomic with mass $|K_i|_{d-1}$ at each n_i,

$$\sigma_K = \sum_{i=1}^m |K_i|_{d-1}\delta_{n_i},$$

and if $K = \mathbb{B}$ is the d-dimensional unit ball, then σ_K simply coincides with the standard (unnormalized) uniform surface area measure $\sigma_K(B) = |B|_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)}\sigma(B)$.

Recall that for a convex body, $K \subset \mathbb{R}^d$, the *support function* $h_K(u)$ of K takes the form

$$h_k(u) = \sup_{v\in K}\langle u, v\rangle.$$

Given two convex bodies K and L, and $p \geq 1$, define

$$V_p(K, L) = \frac{p}{d}\lim_{\epsilon\to 0}\frac{|K +_p \epsilon L| - |K|}{\epsilon},$$

where $K +_p \epsilon L$ is the convex body with support function $h_{K+_p\epsilon L}(u)$ satisfying

$$h_{K+_p\epsilon L}(u)^p = h_K(u)^p + \epsilon h_L(u)^p.$$

Note that for $L = \mathbb{B}_d$ is the unit ball and $p = 1$, the above quantity is just the definition of the surface area of K. In general, $V_p(K, L)$ is known as the *L_p-mixed volume of K and L*. The following alternative integral representation for $V_p(K, L)$ is known

$$V_p(K, L) = \frac{1}{d} \int_{\mathbb{S}^{d-1}} h_L(u)^p d\sigma_K^p(u),$$

where $d\sigma_K^p(u) = h_K(u)^{1-p} d\sigma_K(u)$, so that in particular $d\sigma_K^1(u) = d\sigma_K(u)$.

Now, call a probability measure μ supported on $\mathbb{S}^{d-1}$ admissible, if it is symmetric and not concentrated on a subspace. A classical result which follows from Minkowski's theorem, says that any admissible measure can be realized as the surface area measure of a symmetric convex body; see more in [128, Ch. 7].

The *projection body* ΠK of a convex body K is defined to be a body such that for each $u \in \mathbb{S}^{d-1}$

$$h_{\Pi K}(u) = \left| K | u^\perp \right|_{d-1},$$

that is, the support function of ΠK equals the volume of the projection of K onto the hyperplane orthogonal to u [20]. Since

$$\left| K | u^\perp \right|_{d-1} = \frac{1}{2} \int_{\mathbb{S}^{d-1}} |\langle u, v \rangle| d\sigma_K(v),$$

the identities

$$\begin{aligned} I_{|t|}(\sigma_K) &= \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} |\langle u, v \rangle| \, d\sigma_K(u) d\sigma_K(v) = 2 \int_{\mathbb{S}^{d-1}} \left| K | u^\perp \right|_{d-1} d\sigma_K(u) \\ &= 2 \int_{\mathbb{S}^{d-1}} h_{\Pi K}(u) \, d\sigma_K(u) = 2d \, V_1(K, \Pi K) \end{aligned}$$

finally establish the connection between L_1-mixed volumes and 1-frame energies.

Our main theorem, Theorem 2.1.1, shows that all minimizers of $I_{|t|^p}(\mu)$ over probability measures are admissible when a corresponding tight design exists, as this measure is both discrete and can be taken to be symmetric. From this, we obtain what appears to be a new observation, namely the following:

Proposition 2.7.1. The minimum of the quantity

$$\frac{V_1(K, \Pi K)}{|\partial K|^2}$$

over all symmetric convex bodies in $\mathbb{R}^d$ is achieved when K is a cube.

Indeed, it is easy to see that, when K is a cube, the surface measure σ_K is equally distributed on the vertices of a cross-polytope, which minimizes the p-frame energy for $p = 1$.

One may also define L^p-intersection bodies $\Pi_p K$ [95, 94] in a similar fashion and obtain analogous relations for other values of p. Doing so allows one to infer similar statements for $V_p(K, \Pi_p K)/|\partial K|^2$ for the several dimensions and ranges of p considered in this manuscript (for which tight designs exist), as well as pose conjectures corresponding to the numerically obtained minimizers. We anticipate, in particular, in accordance with the discreteness conjecture, that whenever p is not an even integer, this quantity is always minimized by a convex body which is polyhedral (with discrete surface measure).

2.8 Other linear programming applications

2.8.1 Other energy problems

We now discuss some problems related to minimization of p-frame energies and other energies with degree M absolutely monotonic potentials. For $p \notin 2\mathbb{N}$, the potential functions $f(t) = \frac{1}{2^{p/2}} \cdot (1+t)^{p/2}$, corresponding to the p-frame energy, have the property that not only their derivatives switch signs for large enough orders, but also the coefficients in their Jacobi expansion have alternating signs. While the proof of optimality depended heavily on the former, we look into the latter property now.

In a sense, the most natural polynomial potential functions to consider when approximating $f(t)$

are of the form

$$g(t) = \sum_{m=0}^{k} \widehat{f}_m C_m(t) - \beta C_{k+1}(t), \tag{2.8.1}$$

where $\widehat{f}_m, \beta \geq 0$. Because any earlier truncation of function f is positive definite, so that $I_f(\mu)$ is minimized by surface measure, the point at which the first negative coefficient comes in is the first interesting truncation to consider. At first glance, it may seem that minimizers of $I_g(\mu)$ might act like those of $I_f(\mu)$. When β is too large however, this cannot be true, for in this case a single Dirac mass $\nu = \delta_x$ gives

$$I_g(\nu) = g(\tau(x,x)) = \sum_{m=0}^{k} \widehat{f}_m - \beta,$$

which can be smaller than the value obtained on any other measure. Instead of looking at the energy with potential g, we shall considering the limiting problem of constrained optimization

$$\max_{\mu \in \mathcal{P}(\Omega)} \int_\Omega \int_\Omega C_{k+1}(\tau(x,y)) d\mu(x) d\mu(y) \text{ s.t. } \int_\Omega \int_\Omega C_j(\tau(x,y)) d\mu(x) d\mu(y) = 0,\ j = 1, ..., k, \tag{2.8.2}$$

which is again minimized by tight designs, as the below argument shows.

Theorem 2.8.1. If a tight k-design $\mathcal{C}$ in Ω exists, then the measure $\mu_{\mathcal{C}}$ which distributes mass evenly among the points of $\mathcal{C}$ solves the optimization problem (2.8.2) over probability measures.

Proof. Set $f = C_{k+1}$. If $k = 2m$, we construct the polynomial h by applying Hermite interpolation to f at $t = 1$, and to f and f' at the other m values of $\mathcal{A}(\mathcal{C}) = \{\tau(x,y) | \, x, y \in \mathcal{C}, x \neq y\}$, so that $\deg h \leq 2m = k$. When $k = 2m-1$, i.e. $\mathcal{C}$ contains antipodal pairs, we apply interpolation of order 1 at $t = \pm 1$ and of order 2 at the other $m-1$ values of $\mathcal{A}(\mathcal{C})$, resulting in $\deg h \leq 1 + 2(m-1) = 2m - 1 = k$. The remainder formula (2.3.1) then gives that the difference

$$f(t) - h(t) = \frac{f^{(k+1)}(\xi)}{(k+1)!}(t-1) \cdot \begin{cases} \prod\limits_{\alpha \in \mathcal{A}(\mathcal{C}) \setminus \{1\}} (t-\alpha)^2 \\ \prod\limits_{\alpha \in \mathcal{A}(\mathcal{C}) \setminus \{\pm 1\}} (t-\alpha)^2 \cdot (t+1) \end{cases}$$

is non-positive for $t \in [-1,1]$. This holds because $f^{(k+1)}(\xi) > 0$, as it is simply the leading coefficient of $f = C_{k+1}$. Since h is a polynomial of degree k, the constraints in (2.8.2) imply that for any admissible $\mu \in \mathcal{P}(\Omega)$, $I_h(\mu) = \widehat{h}_0 = I_h(\sigma)$. We therefore obtain

$$I_f(\mu) \leq I_h(\mu) = I_h(\sigma) = I_h(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}),$$

where the penultimate equality relies on the fact that $\mathcal{C}$ is a k-design, and the last one follows from interpolation. $\square$

Note that the argument for uniqueness applies for the above problem, much as it did in the case of degree M absolutely monotonic functions f. The difference lies in the fact that here the design condition arises from the constraints.

Recall that the last chapter showed that for both problem (2.8.2) above and the problem of minimizing g-energy for g as in (2.8.1), there exist finitely supported minimizing measures. Further, in both cases, in addition to the existence of a discrete minimizer, one can obtain quantitative upper bounds on the support size in terms of the number of constraints.

2.8.2 Causal variational principle

Define the kernel

$$\mathcal{L}(t) = \mathcal{L}_\tau(t) := \max\{0, 2\tau^2(1+t)(2-\tau^2(1-t))\}. \tag{2.8.3}$$

for $\tau > 0$. The minimization problem for the energy

$$I_{\mathcal{L}}(\mu) = \int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \mathcal{L}(x \cdot y) d\mu(x) d\mu(y) \tag{2.8.4}$$

is known as the *causal variational principle* on the sphere and is connected to relativistic quantum field theory. It is conjectured in [53] that all the minimizers of (2.8.4) are discrete whenever $\tau > \sqrt{2}$ based on numerical evidence (it is also conjectured that there exist discrete minimizers for $\tau \geq 1$).

Here we confirm this conjecture for two values of $\tau > 0$, for which we can show that the cross-polytope or orthoplex and the icosahedron indeed minimize the energy. These minimizing measures were suggested by numerical experiments in [53].

Cross-polytope: $\tau = \sqrt{2}$

When $\tau = \sqrt{2}$, we have

$$\mathcal{L}(t) = \max\{0, 8t^2 + 8t\},$$

and thus $\mathcal{L}(0) = 0$. Define the measure

$$\nu = \frac{1}{6}\sum_{i=1}^{3}\left(\delta_{e_i} + \delta_{-e_i}\right),$$

where $\{e_1, e_2, e_3\}$ is an orthonormal basis of $\mathbb{R}^3$, i.e. $d\nu$ is a measure whose mass is equally concentrated in the vertices of a cross-polytope. Then we have,

Proposition 2.8.2. The measure ν is a minimizer for the energy, $I_{\mathcal{L}}$, over probability measures on $\mathbb{S}^2$ for $\tau = \sqrt{2}$.

Icosahedron: $\tau^2 = \dfrac{2\sqrt{5}}{\sqrt{5}-1}$

This value of τ is chosen so that $\mathcal{L}_\tau(1/\sqrt{5}) = 0$. Let $\mathcal{C} \subset \mathbb{S}^2$ be the vertices of a regular icosahedron and let

$$\nu = \frac{1}{12}\sum_{x\in\mathcal{C}}\delta_x$$

be the uniform measure on the vertices of the icosahedron.

Proposition 2.8.3. The measure ν is a minimizer for the energy, $I_{\mathcal{L}}$, over probability measures on $\mathbb{S}^2$ for $\tau^2 = \frac{2\sqrt{5}}{\sqrt{5}-1}$.

The proof of Propositions 2.8.2 and 2.8.3 is another application of the linear programming framework, which in this case is particularly straightforward, since, unlike the previous sections, a single auxiliary function must be constructed to certify the solution. We postpone the details to the appendix, see Section A.1.3.

2.9 Further remarks

We have many remaining questions about the p-frame energies, and many curiosities were brought to our attention through our numerical study. One immediate question concerns uniqueness of the 600-cell as a minimizer for $\mathbb{RP}^3$ and $p \in (8, 10)$, which we expect to hold. In Section 2.3.5, we mentioned that tight designs, generally, are not unique (not even up to unitary equivalence). This is known to be true in particular for SIC-POVM's in $\mathbb{C}^3$ through the characterization of all SIC-POVM's in this dimension in [142]. It is interesting whether it is more often the case that infinite families arise or that such configurations are isolated, as is known to be the case when $d = 2$ [162].

An interesting observation is that some configurations minimize p-frame energies for a range of p (the 600-cell for example), while others, like the $p = 3$ minimizer in $\mathbb{RP}^7$, do not minimize on an entire range between even integers. When minimizers have the same support for a range $p \in (2k - 2, 2k)$, it indicates that the supporting configuration has to be a weighted k-design.

For the 36 points in $\mathbb{RP}^7$ given as the midpoints of edges of a regular simplex, one can check that the strength of this configuration as a design is too small to satisfy the above condition. Further, the value of the energy for a measure which equally distributes over this set when compared against the surface measure is too large to be a minimizer when p is close to (but less) than four.

We do not expect that the minimizers of p-frame energies are necessarily weighted k-designs, but noticed that many of the configurations which showed up numerically as limit points of the even p values (from below) were smallest known weighted designs. Informally, one might expect for these configurations to have isolated or small support since if the points become too well distributed, the distribution gets "closer" to surface measure which means the averages of the configuration over the negative coefficient terms in the Jacobi expansion of f vanish. Since one wants to maximize such contributions, the vectors might be taken close to a weighted k-design, but just "barely" so.

Some other cases where the support of a minimizer appears to change within even arguments are for $\mathbb{RP}^2$, $p \in (4, 6)$ and $\mathbb{RP}^3$, $p \in (2, 4)$. One might be tempted to suggest that the configurations which show up as minimizers on an interval are universally optimal, but this is not the case. For example, the D_4 root system, which appears to be optimal on $p \in (4, 6)$ for $\mathbb{S}^3$, is not universally optimal [35]. Nonetheless, in the limited numerical experiments which were run outside of the parameters found in Tables 2.1 and 2.2, it appears uncommon that a configuration be optimal on a range of p, and when it does happen, the configuration is highly structured.

This suggests another phenomenon similar to the notion of universal optimality, and we are tempted to conjecture that in the real case for $d > 2$ there are only finitely many configurations which optimize the p-frame energy on a whole range of $p \in [2k - 2, 2k]$.

As was mentioned earlier, we conjecture that all energies with p not an even integer have discrete and only discrete minimizers. Although the results of the previous chapter show p-frame energies cannot contain an open set in the interior of the support of a minimizing measure, we are not familiar with an argument which would rule out the possibility of an arc of a circle being contained in the support of a minimizing measure for p-frame potentials, or non-positive definite truncations of their Jacobi polynomial expansions.

Looking at the tables, one can note that as the value of p increases, for p not even, the support size of a candidate appears to be monotonically increasing. Further, for a fixed dimension, the support size seems to grow polynomially in p. We do not have an explanation for this phenomenon.

One motivating reason for considering the other projective spaces beyond the real case, is the connection with the problem known as Zauner's conjecture, on existence of tight projective 2-designs, these being best known by their alternative name SIC-POVMs. The moment constrained problem considered in Section 2.8 for $k = 2$ has the property that a discrete solution with support size bounded by an explicit function of d exists regardless of whether a tight design exists. Further, the minimizer must be a (weighted) projective 2-design. If a SIC-POVM exists, it must solve this problem or the p-frame energy problem for $p \in (2, 4)$.

Interestingly, it is conjectured [34] from numerical evidence that the property analogous to Zauner's should not hold in the quaternionic setting. If this is true, it is curious what instead should appear as a minimizer.

Finally, we give additional details on how we made the conjectures found in Tables 2.1 and 2.2. The numerical method employed to find conjectured minimizers involved two steps. Early on, we used a quick first order gradient descent method to minimize energies. Afterwards we implemented an arbitrary precision library with a second order method to check our conjectures and test endpoint behavior. [a]

[a]Chapter adapted from [16].

Table 2.1: Optimal and conjectured optimal configurations for p-frame energies on $\mathbb{RP}^{d-1}$. Energies are evaluated in most cases at the odd integer which is the midpoint of the interval given. The range $q-$ configurations are obtained as limiting configurations as p tends to q from below. For these configurations, the energy is evaluated for the even limit value. Among the configurations which are not tight, the 600-cell is the only configuration which is proved to be optimal.

d	N	Energy	Range of p	Tight	Name
2	N	$(*)$	$[2N-4, 2N-2]$	t	regular $2N$-gon
d	d	$1/d$	$[0,2]$	t	orthonormal basis
3	6	0.241202265916660	$[2,4]$	t	icosahedron
3	11	0.142857142857143	$6-$		Reznick design
3	16	0.124867143799450	$[6,8]$		icosahedron and dodecahedron
4	11	0.125000000000000	$4-$		small weighted design
4	24	0.096277507157493	$[4,6]$		D_4 root vectors
4	60	0.047015486159502	$[8,10]$		600-cell
5	16	0.118257675970387	$[2,4]$		hemicube
5	41	0.061838820473855	$[4,6]$		Stroud design
6	22	0.090559619406078	$[2,4]$		cross-polytope and hemicube
6	63	0.042488105634495	$[4,6]$		E_6 and E_6^* roots
7	28	0.071428571428571	$[2,4]$	t	kissing E_8
7	91	0.030645893660944	$[4,6]$		E_7 and E_7^* roots
8	36	0.059098639455782	3		mid-edges of regular simplex
8	120	0.022916666666667	$[4,6]$	t	E_8 roots
23	276	0.011594202898551	$[2,4]$	t	equiangular lines
23	2300	0.002028985507246	$[4,6]$	t	kissing Leech lattice
24	98280	0.000103419439357	$[8,10]$	t	Leech lattice minimal vectors

Table 2.2: Optimal and conjectured optimal configurations for p-frame energies on $\mathbb{CP}^{d-1}$. The energies are evaluated at odd integers.

d	N	Energy	Range of p	Tight	Name
d	d	$1/d$	$[0, 2]$	t	orthonormal basis
3	9	0.222222222222223	$[2, 4]$	t	SIC-POVM
3	21	0.012610934678518	$[4, 6]$		union equiangular lines
4	16	0.146352549156242	$[2, 4]$	t	SIC-POVM
4	40	0.068301270189222	$[4, 6]$	t	Eisenstein structure on E_8
5	25	0.105319726474218	$[2, 4]$	t	SIC-POVM
5	85	0.041997097378053	$[4, 6]$		O_{10} and $W(K_5)$ minimal vectors
6	36	0.080272843473504	$[2, 4]$	t	SIC-POVM
6	126	0.027777777777778	$[4, 6]$	t	Eisenstein structure on K_{12}

Table 2.3: A list of parameters for the known to exist projective tight designs (besides cross-polytopes, SIC-POVMs, and designs in $\mathbb{FP}^1$). Here M denotes the strength of the design, d the dimension of the ambient space $\mathbb{F}^d$, and N is the size of the design.

d	N	M	Inner Products	$\mathbb{F}$	Name
3	6	2	$1/\sqrt{5}$	$\mathbb{R}$	icosahedron
7	28	2	$1/3$	$\mathbb{R}$	kissing configuration for E_8
8	120	3	$0, 1/2$	$\mathbb{R}$	roots of E_8 lattice
23	276	2	$1/5$	$\mathbb{R}$	tight simplex
23	2300	3	$0, 1/3$	$\mathbb{R}$	kissing configuration for Λ_{24}
24	98280	5	$0, 1/4, 1/2$	$\mathbb{R}$	minimal vectors of Λ_{24}
4	40	3	$0, 1/\sqrt{3}$	$\mathbb{C}$	Eisenstein structure on E_8
6	126	3	$0, 1/2$	$\mathbb{C}$	Eisenstein structure on K_{12}
3	15	2	$\sqrt{14}/7$	$\mathbb{H}$	tight simplex
5	165	3	$0, 1/2$	$\mathbb{H}$	quaternionic reflection group
3	27	2	$2\sqrt{13}/13$	$\mathbb{O}$	tight simplex
3	819	5	$0, 1/2, 1/\sqrt{2}$	$\mathbb{O}$	generalized hexagon of order $(2, 8)$

Table 2.4: Comparison of p-frame energies for conjectured optimal configurations on $\mathbb{RP}^{d-1}$ and $\mathbb{CP}^{d-1}$ with LP lower bounds. Energies are evaluated at the odd integer midpoint of the conjectured optimality interval.

d	$\mathbb{F}$	Energy	LP bound	p	Name
3	$\mathbb{R}$	0.1249	0.1248	7	icosahedron and dodecahedron
4	$\mathbb{R}$	0.09628	0.09607	5	D_4 root vectors
5	$\mathbb{R}$	0.1183	0.1170	3	hemicube
5	$\mathbb{R}$	0.06184	0.06169	5	Stroud design
6	$\mathbb{R}$	0.09056	0.08970	3	cross-polytope and hemicube
6	$\mathbb{R}$	0.04249	0.04240	5	E_6 and E_6^* roots
7	$\mathbb{R}$	0.03065	0.03060	5	E_7 and E_7^* roots
8	$\mathbb{R}$	0.05910	0.05852	3	mid-edges of regular simplex
3	$\mathbb{C}$	0.01261	0.01258	5	union equiangular lines
5	$\mathbb{C}$	0.04200	0.04184	5	O_{10} and $W(K_5)$ minimal vectors

Table 2.5: Table of inner products between vectors in parts X_1, X_2 of the new cubature formula of 85-vectors. N counts the number of times a value occurs as an entry in $|X_i'X_j|$, $i, j = 1, 2$.

	$\lvert\langle x, y\rangle\rvert$	N
$\lvert X_1'X_1\rvert$	$0, 1/2, 1$	$540, 1440, 45$
$\lvert X_2'X_2\rvert$	$1/3, 1/\sqrt{3}, 1$	$1080, 480, 40$
$\lvert X_1'X_2\rvert$	$0, 1/\sqrt{3}$	$720, 1080$
$\lvert X_2'X_1\rvert$	$0, 1/\sqrt{3}$	$720, 1080$

Table 2.6: The Gram matrix of the weighted projective 2-design in $\mathbb{RP}^3$ which appears as a minimizer as $p \to 4^-$ along with ordered weights, with each weight corresponding to the vector with inner products given in the adjacent row. In the matrix, a and b are $\frac{\sqrt{5}+1}{6}$ and $\frac{1}{6}\sqrt{(6-2\sqrt{5})}$, respectively.

$$\left[\begin{array}{ccccccccccc|c}
1 & -\frac{2}{3} & a & a & a & a & b & b & b & b & \frac{\sqrt{6}}{6} & \frac{3}{40} \\
-\frac{2}{3} & 1 & -b & -b & -b & -b & -a & -a & -a & -a & \frac{\sqrt{6}}{6} & \frac{3}{40} \\
a & -b & 1 & \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{6}}{6} & \frac{3}{32} \\
a & -b & \frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{6}}{6} & \frac{3}{32} \\
a & -b & \frac{1}{3} & -\frac{1}{3} & 1 & \frac{1}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{6}}{6} & \frac{3}{32} \\
a & -b & -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 1 & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{6}}{6} & \frac{3}{32} \\
b & -a & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & 1 & \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} & -\frac{\sqrt{6}}{6} & \frac{3}{32} \\
b & -a & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & -\frac{\sqrt{6}}{6} & \frac{3}{32} \\
b & -a & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{1}{3} & -\frac{1}{3} & 1 & \frac{1}{3} & -\frac{\sqrt{6}}{6} & \frac{3}{32} \\
b & -a & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 1 & -\frac{\sqrt{6}}{6} & \frac{3}{32} \\
\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & 1 & \frac{1}{10}
\end{array}\right]$$

CHAPTER 3

REPEATED MINIMIZERS OF P-FRAME ENERGIES

3.1 Introduction

In this chapter we focus primarily on discrete energy problems, addressing the problem where one optimizes over a fixed number of points on the sphere. Let $\mathbf{A} = A_{i,j}$ be an $N \times N$ real matrix of rank less than or equal to d, and with ones along the diagonal. The p-frame energy of matrix $\mathbf{A}$ is denoted

$$E_p(\mathbf{A}) = \sum_{i \neq j} |A_{ij}|^p.$$

An interesting question is what the optimizing matrices for $E_p(\mathbf{A})$ are for fixed p, N, and d. Bukh and Cox in [24] recently studied the question of bounding $E_\infty(\mathbf{A}) = \max\{|A_{ij}|\}$ and its consequences. One special case of this problem concerns matrices associated with unit vectors, $\mathbf{X} = \{x_i\}_{i=1}^N \subset \mathbb{R}^d$, in which case $\mathbf{A}$ is the Gram matrix of $\mathbf{X}$ and so is additionally symmetric and positive semi-definite.

As menioned in an earlier chapter, results and conjectures on minimizers of p-frame energies were formulated by Ehler and Okoudjou in [50]. Using the fact that for $d = N$, the minimizer of $E_p(\mathbf{A})$ for $p = 2$ is an orthonormal basis, they show that whenever N is divisible by d and $p \in (0, 2)$, a repeated orthonormal basis is the unique minimizer. Uniqueness here can be understood by considering the energy on projective spaces $\mathbb{RP}^{d-1}$ (and up to symmetry), where the points in $\mathbb{RP}^{d-1}$ may be identified with lines through the origin in $\mathbb{R}^d$.

The problem of minimizing the 1-frame energy was also posed in [166], where it was conjectured that for any N, the repeated orthonormal basis is the unique minimizer. In 1959, Fejes Tóth posed the question [51]: what is the largest sum of non-obtuse angles formed by N lines in $\mathbb{R}^d$? The conjecture stands that for any N the maximum is uniquely attained on a collection of d lines generated by a repeated orthonormal basis and is resolved only for $d = 2$, and for very few cases of N for $d = 3$. The asymptotic result for $d = 3$ is wide open (see [14] and [56] for recent progress). We note that the conjecture about E_1 from [166] immediately follows from the conjecture of Fejes Tóth since $\arccos t \geq \frac{\pi}{2}(1-t)$ for $t \in [0,1]$ with equality holding precisely at $t = 0$ and $t = 1$.

In this chapter, we develop new methods for finding lower bounds on $E_p(\mathbf{A})$, based on the framework of Bukh and Cox from [24]. Doing so allows us to prove new general bounds for $E_p(\mathbf{A})$ when $p < 2$. Such bounds are sharp in some cases, particularly, for $p = 1$ and $N \in [d+1, 2d]$. We also give sharp bounds for $N = d + m$ and $p \in [1, 2\log\frac{2m+1}{2m}/\log\frac{m+1}{m}]$, where $1 \leq m < d$, thus partially confirming a conjecture from [32].

Although everything in Sections 3.2-3.3 is formulated in the real case, all observations and proofs there work for matrices of complex numbers or quaternions without any changes. Our methods work for general matrix optimization problems, so most of our results will be formulated for matrices. However, we slightly abuse terminology when talking about vector sets instead of their Gram matrices while speaking of $E_p(\mathbf{A})$.

In Section 3.4, we prove that the p-frame energy for unit vectors in the plane is minimized by repeated orthonormal bases for any number of vectors if $p \in [1, 1.3]$. In Section 3.5 we discuss possible generalizations of the results of the paper and motivations behind them connected with ideas from compressed sensing.

3.2 Auxiliary problems and tight frames

Bukh and Cox in [24] introduced a method for deriving new packing bounds for projective codes. In our related approach we use the notion of a tight frame, defined by the equality in equation 1.1.5.

Using the tight frame condition (1.1.5) and comparing coefficients for all d components of x, one can conclude that $\sum_{i=1}^{N}\|y_i\|^2 = Cd$. It is convenient to use the normalization $C = \frac{1}{d}$ for frames as above, so that the Hilbert-Schmidt norm of the $d \times N$ matrix $\mathbf{Y}$, with column vectors $\{y_i\}_{i=1}^N$, is normalized to be 1,

$$\|\mathbf{Y}\|_{\mathrm{HS}}^2 = \sum_{i=1}^{N}\|y_i\|^2 = 1. \tag{3.2.1}$$

In the next two lemmas we collect instruments for computing new lower bounds for discrete p-frame energies. The first makes a connection between kernels of matrices and associated tight frames. We introduce the notation $f_{c,p}(t) = \left(\frac{t}{c-t}\right)^{\frac{p}{2}}$, to be used in the second lemma. We also introduce the optimization problem,

$$M(c,p,N) = \min \left\{ \sum_{i=1}^{N} f_{c,p}(t_i) \middle| \sum_{i=1}^{N} t_i = 1,\ t_i \in [0,c) \right\}, \tag{3.2.2}$$

where $p > 0$ and $c > 1/N$. Clearly, this optimization problem is properly defined.

Lemma 3.2.1. For any real $N \times N$ matrix $\mathbf{A}$ of rank d, $N \geq d+1$, with unit diagonal elements, there exists a tight frame $\{y_1, y_2, \ldots, y_N\} \subset \mathbb{R}^{N-d}$ with the frame constant $\frac{1}{N-d}$ such that $\operatorname{Ker} \mathbf{A}$ consists of all vectors of the form $(\langle y, y_1\rangle, \ldots, \langle y, y_N\rangle)$ with $y \in \mathbb{R}^{N-d}$.

Proof. $\operatorname{Ker} \mathbf{A}$ is $(N-d)$-dimensional so there is a linear mapping $L : \mathbb{R}^{N-d} \to \mathbb{R}^N$ whose image is $\operatorname{Ker} \mathbf{A}$. For each of N components, L is a linear functional so it may be represented as $L_i(y) = \langle y, z_i\rangle$. We note that for any non-singular mapping $D : \mathbb{R}^{N-d} \to \mathbb{R}^{N-d}$, the image of the mapping $L \circ D$ is $\operatorname{Ker} \mathbf{A}$ as well. The quadratic form $\sum_{i=1}^{N} \langle y, z_i\rangle^2$ is positive definite, and so by choosing a suitable D, we can transform $\{z_1, z_2, \ldots, z_N\}$ into $\{y_1, y_2, \ldots, y_N\}$ so that $\sum_{i=1}^{N} \langle y, y_i\rangle^2 = \frac{1}{N-d}\langle y, y\rangle$. So, we obtain the condition 1.1.5, and $\{y_i\}_{i=1}^{N}$ is a tight frame. $\square$

The construction in Lemma 3.2.1 is due to Bukh and Cox [24] who used it for obtaining new packing bounds for projective codes. It also can be interpreted as a tight frame representative of a Gale dual to the matrix A (see [63] for more details about this interpretation).

Lemma 3.2.2. For any real $N \times N$ matrix $\mathbf{A}$ of rank d, $N \geq d+1$, with unit diagonal elements,

$$E_p(\mathbf{A}) \geq M\left(\frac{1}{N-d}, p, N\right) \text{ if } 1 \leq p \leq 2,$$

$$E_p(\mathbf{A}) \geq (N-1)^{1-\frac{p}{2}} M\left(\frac{1}{N-d}, p, N\right) \text{ if } p \geq 2$$

Proof. By Lemma 3.2.1, there exists a tight frame $\{y_1, y_2, \ldots, y_N\} \subset \mathbb{R}^{N-d}$ such that Ker $\mathbf{A}$ is the set of all vectors $(\langle y, y_1\rangle, \ldots, \langle y, y_N\rangle)$ for some $y \in \mathbb{R}^{N-d}$ and $\sum_{i=1}^{N} |y_i|^2 = 1$. Taking $y = y_i$ and using the kernel condition for row i, we get

$$\langle y_i, y_i\rangle + \sum_{j \neq i} A_{ij} \langle y_i, y_j\rangle = 0.$$

Then for any $1 \leq i \leq N$,

$$\langle y_i, y_i\rangle \leq \sum_{j\neq i} |A_{ij}||\langle y_i, y_j\rangle| \leq \left(\sum_{j\neq i} |A_{ij}|^p\right)^{\frac{1}{p}} \left(\sum_{j\neq i} |\langle y_i, y_j\rangle|^q\right)^{\frac{1}{q}},$$

by Hölder's inequality for $\frac{1}{p} + \frac{1}{q} = 1$ (for $q = \infty$, $\left(\sum_{j\neq i} |\langle y_i, y_j\rangle|^q\right)^{\frac{1}{q}} = \max_{j\neq i} |\langle y_i, y_j\rangle|$).

By monotonicity of norms $\|\cdot\|_p$ in p and Hölder's inequality (for vectors in $\mathbb{R}^{N-1}$), $\|x\|_q \leq \|x\|_2$ for $q \geq 2$, while $\|x\|_q \leq (N-1)^{\frac{1}{q}-\frac{1}{2}} \|x\|_2$ when $q \leq 2$. Hence,

$$\langle y_i, y_i\rangle \leq \left(\sum_{j\neq i} |A_{ij}|^p\right)^{\frac{1}{p}} \left(\sum_{j\neq i} \langle y_i, y_j\rangle^2\right)^{\frac{1}{2}} \quad \text{if } p \leq 2, \text{ and,}$$

$$\langle y_i, y_i\rangle \leq (N-1)^{\frac{1}{2}-\frac{1}{p}} \left(\sum_{j\neq i} |A_{ij}|^p\right)^{\frac{1}{p}} \left(\sum_{j\neq i} \langle y_i, y_j\rangle^2\right)^{\frac{1}{2}} \quad \text{if } p \geq 2.$$

At this point we use the tight frame condition for y_i, i.e. $\sum_{j\neq i} \langle y_i, y_j\rangle^2 = \frac{1}{N-d}\langle y_i, y_i\rangle - \langle y_i, y_i\rangle^2$, and denote $\langle y_i, y_i\rangle$ by t_i to arrive finally at the inequalities:

$$\left(\sum_{j\neq i} |A_{ij}|^p\right)^{\frac{1}{p}} \geq \left(\frac{t_i}{\frac{1}{N-d} - t_i}\right)^{\frac{1}{2}} \quad \text{if } p \leq 2, \text{ and,}$$

$$\left(\sum_{j\neq i} |A_{ij}|^p\right)^{\frac{1}{p}} \geq (N-1)^{\frac{1}{p}-\frac{1}{2}} \left(\frac{t_i}{\frac{1}{N-d} - t_i}\right)^{\frac{1}{2}} \quad \text{if } p \geq 2.$$

Taking powers, noting $\sum_{i=1}^{N} t_i = 1$, and summing these inequalities over all i, we obtain the conclusion of the lemma. $\square$

3.3 New lower bounds for the p-frame energy

As a first application of Lemma 3.2.2, we give a new proof of the result from [114] (also Proposition 3.1 in [50]).

Proposition 3.3.1. For any $p \geq 2$ and any real $N \times N$ matrix $\mathbf{A}$ of rank d, $N \geq 2$, with unit diagonal elements,

$$E_p(\mathbf{A}) \geq N(N-1)\left(\frac{N-d}{d(N-1)}\right)^{\frac{p}{2}}.$$

Proof. For $N = d$, the right-hand side is 0. We assume $N \geq d+1$ for the rest of the proof.

For $p \geq 2$, $f_{c,N}(t) = \left(\frac{t}{c-t}\right)^{\frac{p}{2}}$ is convex on $[0, c)$. Due to Jensen's inequality, this implies

$$M\left(\frac{1}{N-d}, p, N\right) = N f_{\frac{1}{N-d},N}\left(\frac{1}{N}\right) = N\left(\frac{N-d}{d}\right)^{\frac{p}{2}}.$$

Together with Lemma 3.2.2 this completes the proof. $\square$

It is straightforward to check that when $p > 2$, the only case in which the inequality of Proposition 3.3.1 is exact, holds when $\mathbf{Y} = \{y_1, \ldots, y_N\}$ is a tight frame in $\mathbb{R}^{N-d}$ which satisfies that $|y_i|$ is constant for all i and $|\langle y_i, y_j\rangle|$ is also constant for all $i \neq j$. In other words equality holds in Proposition 3.3.1 if and only if $\mathbf{Y}$ is an *equiangular tight frame* (ETF). In view of $\mathbf{Y}$ as an ETF, matrix $\mathbf{A}$ is then the Gram matrix of the d-dimensional ETF known as the *Naimark complement* or *Gale dual* to $\mathbf{Y}$ (see, for instance, [30] and [34] for more details about Naimark complements and Gale duality of equiangular tight frames).

There are several interesting properties of ETFs but the two most fundamental are that they are precisely the equality achieving systems of vectors for the *Welch bound*, and the maximum size N of such systems is limited by *Gerzon's bound*.

The Welch bound gives a lower bound for the *coherence* of a system of unit vectors namely, for unit vectors $\{\varphi_i\}_{i=1}^N \subset \mathbb{R}^d$ or $\mathbb{C}^d$,

$$\max_{i \neq j} |\langle \varphi_i, \varphi_j \rangle| \geq \sqrt{\frac{N-d}{d(N-1)}}.$$

This bound is one example of several other bounds which limit how spread out the one-dimensional subspaces corresponding to each vector may be [154]; see [92] for similar bounds and their derivation from a linear programming approach.

Gerzon's bound [88] limits the size of an ETF, and states in the real and complex case respectively,

$$N \leq \binom{d+1}{2} \text{ and } N \leq d^2.$$

We call ETFs attaining this bound *maximal*. There are known maximal ETFs for $d = 1, 2, 3, 7, 23$ only (recall the non-trivial ones appeared in Table 2.1). We discuss maximal ETFs further in connection with Theorem 3.5.1 in Section 3.5. Using the lemmas from the previous section, we now give another observation on the relation between optimizing $E_p(\mathbf{A})$ and the problem $M(c, p, N)$.

Theorem 3.3.2. For any $1 \leq p < 2$ and any real $N \times N$ matrix $\mathbf{A}$ of rank d with unit diagonal elements,

$$E_p(\mathbf{A}) \geq \frac{2(N-d)}{p^{\frac{p}{2}}(2-p)^{\frac{2-p}{2}}}.$$

Proof. For $N = d$, the right-hand side is 0. We assume $N \geq d+1$ for the rest of the proof.

$f_{\frac{1}{N-d},N}(t)/t$ is minimized on $(0, \frac{1}{N-d})$ at $t_0 = \frac{2-p}{2(N-d)}$. Hence,

$$f_{\frac{1}{N-d},N}(t) \geq \frac{2(N-d)}{p^{\frac{p}{2}}(2-p)^{\frac{2-p}{2}}} t, \text{ and so,}$$

$$M\left(\frac{1}{N-d}, p, N\right) \geq \frac{2(N-d)}{p^{\frac{p}{2}}(2-p)^{\frac{2-p}{2}}} \sum_{i=1}^{N} t_i = \frac{2(N-d)}{p^{\frac{p}{2}}(2-p)^{\frac{2-p}{2}}}.$$

The final bound then follows from Lemma 3.2.2. □

When taking $p = 1$ in Theorem 3.3.2, we get $E_1(\mathbf{A}) \geq 2(N-d)$. For N in the range $d+1 \leq N \leq 2d$, we thus obtain the bound conjectured in [166] from Theorem 3.3.2. We formulate it here as a simple statement about angles between lines in Euclidean spaces where it is understood that such angles are restricted to lie in $[0, \pi/2]$.

Corollary 3.3.3. The sum of cosines of all pairwise angles between N lines in $\mathbb{R}^d$ is at least $N-d$. For $N \in [d, 2d]$, the bound is sharp and the unique minimizer is the set of N lines forming a repeated orthonormal basis.

As hinted in the discussion [166], Corollary 3.3.3 may be proven by induction. For the sake of completeness, we provide such a proof here as well.

Alternative proof of Corollary 3.3.3. We choose a unit vector in the direction of each of the N lines and construct an $N \times N$ Gram matrix for the chosen vectors. The matrix has rank no greater than d so, by the Gershgorin circle theorem, any $(d+1) \times (d+1)$ diagonal minor of the matrix will have at least one row whose sum of absolute values of non-diagonal entries is at least 1. The inductive step consists then in finding one row like this and using the inductive hypothesis for the $(N-1) \times (N-1)$ diagonal minor obtained by deleting this row and the column symmetric to it from the matrix. $\square$

It is unkown how to extend this short proof to a more general problem of finding lower bounds for the 1-frame energy of matrices that is covered by Theorem 3.3.2. The proof of Corollary 3.3.3 does not seem to work for non-symmetric matrices. We also note that Theorem 3.3.2 implies the same bound $2(N-d)$ for $E_p(\mathbf{A})$ when $p \in (0, 1)$.

For the case of $N = d + 1$, Chen, Gonzales, Goodman, Kang, and Okoudjou [32] posed a conjecture for the minimum of the p-frame energy for all $p \in (0, 2)$. They conjectured that a global minimum is necessarily formed by $k + 1$ unit vectors whose endpoints form a regular k-dimensional simplex and $N - k - 1$ vectors that are pairwise orthogonal and orthogonal to the subspace of the regular simplex. In particular, their conjecture states that for $p < \frac{\ln 3}{\ln 2} \approx 1.58496$, the minimum is 2 and attained only on the repeated orthogonal basis with $d + 1$ vectors.

We now study a more general problem of optimizing over $d+m$ vectors, $1 \leq m < d$, and, using Lemma 3.2.2, prove that the repeated orthonormal basis minimizes E_p for $p \in [1, p_m]$. In particular, for $m = 1$, our results confirm the conjecture from [32] for p in the range $p \leq 2(\frac{\ln 3}{\ln 2} - 1) \approx 1.16993$.

Theorem 3.3.4. For $p \in [1, 2\log\frac{2m+1}{2m}/\log\frac{m+1}{m}]$, $1 \le m < d$ and a real $(d+m)\times(d+m)$ matrix $\mathbf{A}$ of rank d with ones along the diagonal,

$$E_p(\mathbf{A}) = \sum_{i\neq j}|A_{i,j}|^p \ge \ 2m.$$

The following lemma is used in the proof of Theorem 3.3.4.

Lemma 3.3.5. Set $\alpha = \frac{1}{m}\left(\frac{1}{2}-\frac{p}{4}\right)$. For $p \in [1,2]$, $M(\frac{1}{m}, p, N)$ is minimized for t_j of the form

(i) $t_1 = \cdots = t_k = \frac{1}{k},\ t_{k+1} = \cdots = t_n = 0$, where $\frac{1}{k} \ge \alpha$, or,

(ii) $t_1 = \cdots = t_k = x$, $t_{k+1} = 1-kx$, $t_{k+2} = \cdots = t_N = 0$, where $x \ge \alpha$, $0 < 1-kx < \alpha$.

Proof. Computing the second derivative of $f_{1/m,p}(t)$, we see it is concave on $[0,\alpha]$ and convex on $[\alpha, 1)$ where $\alpha = \frac{1}{m}\left(\frac{1}{2}-\frac{p}{4}\right)$. All t_i lying in $[0,\alpha]$ may be moved to the endpoints of the interval, except for at most one number, while keeping their sum constant and minimizing the sum of values of $f_{1,p}$ (this follows, for instance, from the Karamata inequality, see [71, pg 89]). After this we may apply Jensen's inequality for all numbers from $[\alpha, 1)$ and assume they are all equal. The resulting minimizer is then necessarily one of the two types: 1) $t_1 = \ldots = t_k = \frac{1}{k}$, $t_{k+1} = \ldots = t_N = 0$, where $\frac{1}{k} \ge \alpha$, 2) $t_1 = \ldots = t_k = x$, $t_{k+1} = 1-kx$, $t_{k+2} = \ldots = t_N = 0$, where $x \ge \alpha$ and $0 < 1-kx < \alpha$. □

We now follow with a proof of Theorem 3.3.4.

Proof. Set $p_m = 2\log\frac{2m+1}{2m}/\log\frac{m+1}{m}$ and $q_m = \frac{p_m}{2}$. Clearly, it is sufficient to prove the lower bound for $p = p_m$ only. We use Lemma 3.2.2 and show that $M(\frac{1}{m}, p, N) \ge 2m$. Consider the first case in the above lemma, so that

$$t_1 = \cdots = t_k = \frac{1}{k},\ t_{k+1} = \cdots = t_n = 0,$$

where $\frac{1}{k} \geq \alpha = \frac{1}{m}\left(\frac{1}{2} - \frac{p_m}{4}\right)$. In this case, we need to minimize the value

$$k f_{1/m,p_m}\left(\frac{1}{k}\right) = k\left(\frac{m}{k-m}\right)^{\frac{p_m}{2}}.$$

The real function

$$F_m(x) = x\left(\frac{m}{x-m}\right)^{\frac{p_m}{2}} \tag{3.3.1}$$

for $x > m$ has exactly one local minimum. The degree p_m was specifically chosen so that $F_m(2m) = F_m(2m+1) = 2m$. Then by Rolle's theorem, the local minimum of $F_m(x)$ lies in $[2m, 2m+1]$. The minimum of $F_m(x)$ for natural values of x, $x > m$, is, therefore, attained on $2m$ and $2m+1$ and is equal to $2m$.

In the second case, $x < \frac{1}{k}$ and $x \geq \alpha = \frac{1}{m}\left(\frac{1}{2} - \frac{p_m}{4}\right)$. It is straightforward to show that $p_m < \frac{4m+2}{4m+1}$ for all natural m. Subsequently $k < \frac{1}{\alpha} < 4m+1$ so that k can take (integer) values only in $[m, 4m]$. To show $E_{p_m} \geq 2m$ it suffices then to show for all $m \leq j \leq 4m$, and all x in $I = (\frac{1}{j+1}, \frac{1}{j})$ that the function

$$g_j(x) = j\left(\frac{mx}{1-mx}\right)^{q_m} + \left(\frac{m(1-jx)}{1-m(1-jx)}\right)^{q_m},$$

satisfies $g_j(x) \geq 2m$. This will be demonstrated using properties specific to $g_j(x)$, namely that the function has at most one critical point, $g_j'(x) = 0$, inside the interval I. Taking derivatives,

$$g_j'(x) = q_m j m\left[\left(\frac{mx}{1-mx}\right)^{q_m-1}\frac{1}{(1-mx)^2} - \left(\frac{m(1-jx)}{1-m(1-jx)}\right)^{q_m-1}\frac{1}{(1+m(-1+jx))^2}\right],$$

so that $g_j'(x) = 0$ gives

$$\begin{aligned}
\left(\frac{x(1+m(-1+jx))}{(1-mx)(1-jx)}\right)^{q_m-1} &= \frac{(1-mx)^2}{(1+m(-1+jx))^2} \\
\left(\frac{x(1+m(-1+jx))}{(1-mx)(1-jx)}\right)^{q_m+1} &= \frac{x^2}{(1-jx)^2} \\
\frac{1+m(-1+jx)}{1-mx} &= \left(\frac{x}{(1-jx)}\right)^{\frac{2}{q_m+1}-1} \\
\frac{1-mx}{1+m(-1+jx)} &= \left(\frac{x}{(1-jx)}\right)^{1-\frac{2}{q_m+1}}.
\end{aligned}$$

Calling the function on the left in the above expression $f(x)$ and the function on the right $g(x)$,

$$f''(x) = \frac{2j(1+j-m)m^2}{(1+m(-1+jx))^3} > 0 \text{ on } I,$$

while letting $\gamma = 1 - \frac{2}{q_m+1}$,

$$g''(x) = \frac{\gamma(\frac{x}{1-jx})^{\gamma}(\gamma - 1 + 2jx)}{x^2(jx-1)^2} < 0 \text{ on } I,$$

since $\gamma < 0$. Thus $f(x)$ is convex on I, while $g(x)$ is concave on I. Since $f(\frac{1}{j+1}) = g(\frac{1}{j+1})$ and $f'(\frac{1}{j+1}) \leq g'(\frac{1}{j+1})$, when $j < 4m$, it must be the case then that $f(x) = g(x)$ for exactly one point $x \in I$, ($x \neq \frac{1}{j+1}, \frac{1}{j}$). Note that when $j = 4m$ there are no critical points in I. Now,

$$g_j'\left(\frac{1}{j+1}\right) = 0 \text{ and } \lim_{x \to \frac{1}{j}} g_j'(x) = -\infty.$$

Thus the critical points correspond to local maxima of $g_j(x)$ and it suffices to check the value of $g_j(x)$ at the endpoints in I for each $m \leq j \leq 4m$ to establish the desired lower bound. These values are

$$g_j\left(\frac{1}{j+1}\right) = (1+j)\left(\frac{m}{1+j-m}\right)^{q_m} = F_m(j+1), \text{ and } g_j\left(\frac{1}{j}\right) = j\left(\frac{m}{j-m}\right)^{q_m} = F_m(j),$$

where F_m is the function defined in equation (3.3.1). The minimal value of $F_m(x)$ on natural numbers, $x > m$, as we established earlier, is precisely $2m$. □

Following the proofs of Theorem 3.3.4 and Lemma 3.2.2 it is easy to check that the only minimizer is the repeated orthonormal basis. Theorem 3.3.4 was first announced by the author in [116].

3.4 Minimizing discrete energy on the circle for small p

In this section, we study the problem of minimizing the p-frame energy for collections of unit vectors in the plane. In particular, we show that the repeated orthonormal basis is the minimizer for $p \leq 1.3$. As one of the instruments for our proof, we use the solution of the Fejes Tóth problem mentioned in Section 4.1.

Theorem 3.4.1. Let $x_1, x_2, \ldots, x_N$ be unit vectors in the plane. Then,

$$\sum_{i,j=1}^{N} \arccos|\langle x_i, x_j\rangle| \leq \frac{\pi N^2}{4}, \text{ if } N \text{ is even,}$$

$$\sum_{i,j=1}^{N} \arccos|\langle x_i, x_j\rangle| \leq \frac{\pi (N^2-1)}{4}, \text{ if } N \text{ is odd.}$$

Theorem 3.4.1 was proven in [56]. Several alternative proofs were also obtained in [14].

Theorem 3.4.2. Let $\mathbf{A}$ be a Gram matrix of N unit vectors in the plane. Then for $p \in (0, 1.3]$, $E_p(A) \geq N(N-2)/2$ if N is even and $E_p(A) \geq (N-1)^2/2$ if N is odd.

Proof. Assume $\mathbf{A}$ is the Gram matrix of unit vectors $x_1, x_2, \ldots, x_N$ in the plane.

For any $p \in [0, 2]$, the lower bound on E_p for even N follows immediately from the fact that a repeated orthonormal basis is one of the minimizers of E_2 when the number of vectors is divisible by the dimension (see [50, 134, 148]).

It is sufficient to prove the lower bound for $p = 1.3$ so we consider this case only for the rest of the proof. For odd N, we split our proof into two parts: 1) angles between each pair of vectors are sufficiently far from $\pi/2$; 2) there are vectors that are almost orthogonal. For the first case, we assume that all angles $\arccos|\langle x_i, x_j\rangle|$, $1 \le i, j \le N$, are no greater than 1.34. It is straightforward to check that for any $t \in [0, 1.34]$,

$$\cos^{1.3} t \ge \frac{2}{\pi}\left(\frac{\pi}{2} - t\right).$$

Summing these inequalities for all $t = \arccos|\langle x_i, x_j\rangle|$, $1 \le i, j \le N$, $i \ne j$, we obtain

$$E_{1.3}(\mathbf{A}) \ge N^2 - N - \frac{2}{\pi}\sum_{i,j=1}^{N} \arccos|\langle x_i, x_j\rangle|.$$

Using the solution of the Fejes Tóth problem from Theorem 3.4.1 we conclude

$$E_{1.3}(\mathbf{A}) \ge N^2 - N - \frac{2}{\pi}(N^2-1)\frac{\pi}{4} = \frac{(N-1)^2}{2}.$$

For the second case, we assume that the largest angle among $\arccos|\langle x_i, x_j\rangle|$, $1 \le i, j \le N$, is at least 1.34. Without loss of generality, let one of such angles be $\arccos|\langle x_1, x_2\rangle|$. Our proof will be by induction on odd numbers N. The statement of the theorem is clearly true for $N = 1$. Let N be an odd number greater than 1. Now we will show that for any i, $3 \le i \le N$,

$$|\langle x_1, x_i\rangle|^{1.3} + |\langle x_2, x_i\rangle|^{1.3} \ge 1.$$

We can always switch a vector to its opposite without changing the total energy so we may assume that x_i lies in the angle formed by x_1 and x_2. We assume the angle between x_1 and x_2 is ϑ and x_i forms the angles of ϕ and $\vartheta - \phi$ with x_1 and x_2, respectively. Note that both ϕ and $\vartheta - \phi$ must be less than $\pi/2$, otherwise one of them is closer to $\pi/2$ than ϑ. Without loss of generality, $\phi \le \vartheta/2$. There are two possible options: $\vartheta \le \pi/2$ and $\vartheta > \pi/2$.

For the first option,

$$|\langle x_1, x_i\rangle|^{1.3} + |\langle x_2, x_i\rangle|^{1.3} = \cos^{1.3}\phi + \cos^{1.3}(\vartheta - \phi) \ge \cos^{1.3}\phi + \cos^{1.3}\left(\frac{\pi}{2} - \phi\right) \ge 1.$$

For the second option, $\vartheta \leq \pi - 1.34$ because $\vartheta = \pi - \arccos|\langle x_1, x_2\rangle|$. The angle ϑ is the one closest to $\pi/2$ among all angles formed by the vectors. In particular, $\vartheta - \phi$ cannot be closer to $\pi/2$ so $\vartheta - \phi \leq \pi - \vartheta$. This condition can be rewritten as $\frac{\pi-\phi}{2} \geq \vartheta - \phi$. For the next step we try to minimize $\cos^{1.3}\phi + \cos^{1.3}(\vartheta - \phi)$ by keeping ϕ intact and increasing $\vartheta - \phi$ as much as possible while preserving the conditions $\vartheta - \phi \leq \pi - \phi - 1.34$ and $\vartheta - \phi \leq \frac{\pi-\phi}{2}$. While increasing ϑ, at some moment we reach the point when one of these two inequalities becomes a precise equality. These two possibilities can be described by the two cases depending on the value of ϕ.

For the first case, assume $\frac{\pi-\phi}{2} > 1.34$, i.e. $\phi < \pi - 2.68$. Then

$$\cos^{1.3}\phi + \cos^{1.3}(\vartheta - \phi) \geq \cos^{1.3}\phi + \cos^{1.3}\left(\frac{\pi - \phi}{2}\right) = \cos^{1.3}\phi + \sin^{1.3}\frac{\phi}{2}.$$

The function $\cos^{1.3}\phi + \sin^{1.3}\frac{\phi}{2}$ is at least 1 for $\phi \in [0, \pi - 2.68]$ so the first case is covered.

For the second case, we assume $\frac{\pi-\phi}{2} \leq 1.34$, i.e. $\phi \geq \pi - 2.68$. We know that $\phi \leq \vartheta/2 \leq \frac{\pi-1.34}{2}$. Using the inequality $\vartheta < \pi - 1.34$ again we get that $\vartheta - \phi < \pi - 1.34 - \phi$. This implies

$$\cos^{1.3}\phi + \cos^{1.3}(\vartheta - \phi) \geq \cos^{1.3}\phi + \cos^{1.3}(\pi - 1.34 - \phi).$$

The function $\cos^{1.3}\phi + \cos^{1.3}(\pi - 1.34 - \phi)$ is at least 1 for $\phi \in [\pi - 2.68, \frac{\pi-1.34}{2}]$. Overall, we conclude that $|\langle x_1, x_i\rangle|^{1.3} + |\langle x_2, x_i\rangle|^{1.3} = \cos^{1.3}\phi + \cos^{1.3}(\vartheta - \phi) \geq 1$.

Then, by the induction hypothesis for unit vectors $x_3, \ldots, x_N$,

$$E_{1.3}(\mathbf{A}) \geq \frac{(N-3)^2}{2} + 2\sum_{i=3}^{N}(|\langle x_2, x_i\rangle|^{1.3} + |\langle x_1, x_i\rangle|^{1.3})$$

$$\geq \frac{(N-3)^2}{2} + 2(N-2) = \frac{(N-1)^2}{2}.$$

□

We do not know how to extend this proof to the general case of matrices of rank 2. The value $p = 1.3$ is not the best possible. One can impose all conditions necessary for the proof of Theorem

3.4.2 to work and optimize for p. The numerical value obtained this way is approximately 1.317.

3.5 Discussion

Recently, the conjecture mentioned above from the paper [32] was proved true in [159]. In particular, the range that the orthonormal basis plus a vector minimizes in Theorem 3.3.4 can be increased to the value $p = \log 3/\log 2$. The behavior of the other maximal values of p that similar constructions are expected to minimize for is suggested in the following conjecture (appearing first in [116]).

Conjecture 1. *Let $N = m + kd$ points be given in $\mathbb{S}^{d-1}$, with $1 \leq m < d$, $d \geq 2$, and a Gram matrix $\mathbf{A} \in \mathbb{R}^{N\times N}$. Then there is a value of p_0, independent of dimension d and excess m, such that the repeated orthonormal sequence $\{e_{j \mod d}\}_{j=1}^{N}$ minimizes E_p over all size N systems of unit vectors (with value $E_p(\mathbf{A}) = d(k^2 - k) + 2k$) for $p < p_0$ and the minimum value of $E_p(\mathbf{A})$ satisfies $E_p(\mathbf{A}) < d(k^2 - k) + 2k$ when $p > p_0$. Further $p_0 = p_0(k)$ satisfies $p_0(k) \to 2$ as $k \to \infty$.*

Theorem 3.4.2, can be interpreted as an improvement to Theorem 3.3.4 from the previous section, and partial progress towards the above conjecture. The parameter $p_0 = 1.3$ in Theorem 3.4.2 is the same for all values of k. It might be interesting to find an elementary argument which showed that $p_0(k) \to 2$ in dimension 2, let alone generally.

Theorem 3.3.4 and Conjecture 1 appear to be examples of a more general phenomenon. The direct analogs/extensions of orthonormal bases are regular simplices in the non-projective setting and maximal ETFs in projective spaces. In the first case, the analogous potential function is $f^{\Delta}_{d,p}(t) = |t + \frac{1}{d}|^p$. In the second case, one can view the potential function $f(t) = |t|^p$ as an instance of the more general function $f_{\alpha,p}(t) = |t^2 - \alpha^2|^p$, and the orthonormal basis as an example of an equiangular tight frame ($|\langle x, y\rangle| = \alpha$, for $x \neq y$ with coherence $\alpha = 0$). The problem of minimizing the energies $E^{\Delta}_{d,p}$ and $E_{\alpha,p}$, associated with $f^{\Delta}_{d,p}$ and $f_{\alpha,p}$, respectively, for p close to 0 might be expected to pick out repeated regular simplices and repeated ETFs with coherence α. We conjecture generally:

Conjecture 2. *(i) Let $\mathbf{A} \in \mathbb{R}^{N\times N}$ be the Gram matrix of $N = m + k(d+1)$ points given in $\mathbb{S}^{d-1}$, with $1 \leq m < d+1$, $d \geq 2$, and let $\{\varphi_i\}_{i=1}^{l} \subset \mathbb{R}^d$ be the maximal regular simplex in $\mathbb{S}^{d-1}$. Then there is a value of $p_0 > 0$, such that the repeated regular simplex $\{\varphi_{j \mod l}\}_{j=1}^{N}$ minimizes $E_{d,p}^{\Delta}$ over all size N systems of unit vectors for $p < p_0$.*

(ii) Let $\mathbf{A} \in \mathbb{R}^{N\times N}$ be the Gram matrix of $N = m + kl$ points given in $\mathbb{S}^{d-1}$, with $1 \leq m < l$, $d \geq 2$, and l the size of an ETF with coherence α, $\{\varphi_i\}_{i=1}^{l} \subset \mathbb{R}^d$. Then there is a value of $p_0 > 0$, such that the repeated ETF sequence $\{\varphi_{j \mod l}\}_{j=1}^{N}$ minimizes $E_{\alpha,p}$ over all size N systems of unit vectors for $p < p_0$.

Conjectures 1 and 2 emphasize the possibility of repeated configurations minimizing p-frame or p-frame-type energies among sets of N points for all large enough N. This property may be seen as a strong version of stability of an optimizing set.

The collections of unit vectors $\Phi = \{\varphi_i\}_{i=1}^{l} \subset \mathbb{R}^d$ that, for all $N \geq l$, have a repeated set $\{\varphi_{j \mod l}\}_{j=1}^{N}$ minimizing the energy defined by the potential function f among all $N \times N$ Gram matrices $\mathbf{A}$, also satisfy that the uniform distribution over Φ must solve the problem,

$$\min_{\mu\in\mathcal{P}(\mathbb{S}^{d-1})} I_f(\mu) = \min_{\mu\in\mathcal{P}(\mathbb{S}^{d-1})} \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y\rangle) d\mu(x) d\mu(y), \tag{3.5.1}$$

where $\mathcal{P}(\mathbb{S}^{d-1})$ are Borel probability measures, $\mu(\mathbb{S}^{d-1}) = 1$. For the case of p-frame energies, *tight designs* are examples of configurations such that uniform distributions over them minimize $I_f(\mu)$ over ranges of p [16]. This behavior is slightly different from that conjectured above, as repeated tight designs of size l can only be expected to minimize the discrete energies when $N = kl$, generally.

The existence of a p_0 in these conjectures might be expected in connection with ideas from the field of *compressed sensing*. One should expect that, as $p \to 0$, the solution to this minimization problem is a repeated ETF (as upon vectorizing the Gram matrix, and considering the difference, the sparsest difference arises this way), but Conjecture 2 strengthens this to say that the solution for p sufficiently small is also a repeated ETF.

In connection with these observations we collect further support for the above conjectures for maximal ETFs and the regular simplex, by showing they minimize the associated continuous energies (3.5.1). The second part of the below theorem holds also with the coherence replaced with the corresponding value on a complex maximal ETF, these being known alternatively as *symmetric informationally complete positive operator-valued measures* (SIC-POVMs, see [59] for more details). We give the proof only in the real case, but the same type of argument applies in the complex case.

Theorem 3.5.1. The following statements hold:

(i) The uniform distribution over the vertices of a regular simplex $\{\varphi_i\}_{i=1}^{d+1} \subset \mathbb{S}^{d-1}$ minimizes the continuous energy $I^{\Delta}_{d,p}$ for $f^{\Delta}_{d,p}(t) = |t + \frac{1}{d}|^p$ for all $p \in (0, 2]$.

(ii) Whenever a maximal ETF exists, $\{\varphi_i\}_{i=1}^{M} \subset \mathbb{S}^{d-1}$ (with coherence $\alpha^2 = \frac{1}{d+2}$), the uniform distribution over its points minimizes the continuous energy $I_{\alpha,p}$ for $f_{\alpha,p}(t) = |t^2 - \alpha^2|^p$ for all $p \in (0, 2]$.

Proof. Note that the inequalities

$$\left|\frac{t+\frac{1}{d}}{1+\frac{1}{d}}\right|^p \geq \left|\frac{t+\frac{1}{d}}{1+\frac{1}{d}}\right|^2 \quad \text{and} \quad \left|\frac{t^2-\frac{1}{d+2}}{1-\frac{1}{d+2}}\right|^p \geq \left|\frac{t^2-\frac{1}{d+2}}{1-\frac{1}{d+2}}\right|^2, \tag{3.5.2}$$

hold for $t \in [-1, 1]$. The first inequality implies $I^{\Delta}_{d,p} \geq (1 + \frac{1}{d})^{p-2} I^{\Delta}_{d,2}$ and the equality holds for the uniform distribution over the regular simplex. The second inequality implies $I_{\alpha,p} \geq (1-\frac{1}{d+2})^{p-2} I_{\alpha,2}$ and the equality holds for the uniform distribution over a maximal ETF. It is sufficient then to prove the theorem for $p = 2$.

For the proof in the case $p = 2$, we use the notion of *positive definite functions* on unit spheres defined in Chapter 1. Note that for any positive definite f and any measure μ on $\mathbb{S}^{d-1}$,

$$I_f(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y \rangle) d\mu(x) d\mu(y) \geq 0.$$

Positive definite functions on spheres were characterized by Schoenberg [129]. In particular, t, $t^2 - \frac{1}{d}$, and $t^4 - \frac{6}{d+4}t^2 + \frac{3}{(d+2)(d+4)}$ (Gegenbauer polynomials of degrees 1, 2, 4) are positive definite functions on $\mathbb{S}^{d-1}$.

Since $(t + \frac{1}{d})^2 = (t^2 - \frac{1}{d}) + \frac{2}{d}t + \frac{d+1}{d^2}$,

$$I^{\Delta}_{d,2}(\mu) \geq \frac{d+1}{d^2}.$$

It is easy to check that for the uniform distribution over the regular simplex, $I^{\Delta}_{d,2}$ is precisely $\frac{d+1}{d^2}$.

Using

$$\left(t^2 - \frac{1}{d+2}\right)^2 = \left(t^4 - \frac{6}{d+4}t^2 + \frac{3}{(d+2)(d+4)}\right) + \frac{4(d+1)}{(d+2)(d+4)}\left(t^2 - \frac{1}{d}\right) + \frac{2(d+1)}{d(d+2)^2},$$

we conclude that

$$I_{\alpha,2}(\mu) \geq \frac{2(d+1)}{d(d+2)^2}.$$

Again it is easy to check that the equality is attained on the uniform distribution over the maximal ETF. □

Using the design conditions, one can also show that the configurations from Theorem 3.5.1 are unique minimizers (up to the uniqueness of maximal ETFs in the second case) for the corresponding energies when $p \in (0, 2)$, similarly to how it is done in [16] for the general case of tight designs and p-frame energies. [a]

[a]Chapter adapted from [64].

CHAPTER 4

LATTICES FROM TIGHT FRAMES AND VERTEX TRANSITIVE GRAPHS

4.1 Introduction

Let $\langle\ ,\ \rangle$ be the usual inner product on $\mathbb{R}^k$ and $\|\boldsymbol{x}\|:=\langle\boldsymbol{x},\boldsymbol{x}\rangle^{1/2}$ the Euclidean norm on $\mathbb{R}^k$. For a lattice $L\subset\mathbb{R}^k$ of full rank k (that is a discrete co-compact subgroup of $\mathbb{R}^k$) the *minimal norm* of L is

$$|L|:=\min\{\|\boldsymbol{x}\|: \boldsymbol{x}\in L\setminus\{\boldsymbol{0}\}\},$$

and its set of *minimal* or *shortest vectors* is

$$S(L):=\{\boldsymbol{x}\in L:\|\boldsymbol{x}\|=|L|\}.$$

The *automorphism group* of the lattice L, $\mathrm{Aut}(L)$, is the group of all $k\times k$ real orthogonal matrices that map L to itself. A particularly interesting class of lattices are *eutactic* lattices: a lattice L is called eutactic if its set of minimal vectors $S(L)$ satisfies a eutaxy condition, i.e. there exist positive real numbers $c_1,\dots,c_n$, (called eutaxy coefficients) such that

$$\|\boldsymbol{v}\|^2=\sum_{\boldsymbol{x}\in S(L)} c_i\langle\boldsymbol{v},\boldsymbol{x}_i\rangle^2 \tag{4.1.1}$$

for all $\boldsymbol{v}\in\mathbb{R}^k$. If $c_1=\cdots=c_n$, L is said to be *strongly eutactic*. Eutactic and strongly eutactic lattices are central objects of lattice theory due to their importance in connection with well studied optimization problems. A theorem of Voronoi (1908) asserts that L is a local maximum of the packing density function on the space of lattices in $\mathbb{R}^k$ if and only if L is eutactic and perfect (L is *perfect* if the set $\{\boldsymbol{x}^\top\boldsymbol{x}:\boldsymbol{x}\in S(L)\}$ spans the space of $k\times k$ real symmetric matrices) [151]. More details on eutactic, strongly eutactic and perfect lattices can be found in J. Martinet's book [103].

Two lattices L and M are called *similar*, written $L \sim M$, if $L = \alpha UM$ for a nonzero scalar α and an orthogonal transformation U. Similarity is an equivalence relation on lattices that preserves inner products between vectors (up to the scalar α) and, as a result, lattice's automorphism group; it also gives a bijection between sets of minimal vectors. Consequently, all the geometric properties that we discuss here, such as eutaxy, strong eutaxy and perfection are preserved on similarity classes.

In the papers [26] and [25], lattices generated by equiangular tight frames (ETFs) were studied and examples of strongly eutactic such lattices were constructed. Here we aim to take this discussion further. Let $n \geq k$ and let $\mathcal{F} := \{\boldsymbol{f}_1, \dots, \boldsymbol{f}_n\} \subset \mathbb{R}^k$ be a sequence of vectors, not necessarily distinct, such that $\operatorname{span}_{\mathbb{R}} \{\boldsymbol{f}_1, \dots, \boldsymbol{f}_n\} = \mathbb{R}^k$. Such a set $\mathcal{F}$ is called an (n, k)-*frame*, the name originating in a 1952 paper of Duffin and Schaeffer in connection with their study of nonharmonic Fourier series [49]. A frame $\mathcal{F}$ is called *uniform* if all of its vectors have the same norm. Recall that a frame is called *tight* if there exists a real constant $\gamma > 0$ such that for every $\boldsymbol{v} \in \mathbb{R}^k$

$$\|\boldsymbol{v}\|^2 = \gamma \sum_{i=1}^{n} \langle \boldsymbol{v}, \boldsymbol{f}_i \rangle^2, \tag{4.1.2}$$

and a tight frame is called *Parseval* if $\gamma = 1$: clearly, any tight frame can be rescaled to a Parseval frame. Notice the similarity between this equation and the equation (4.1.1) above. Although the tightness condition (4.1.2) above is well studied in several contemporary branches of mathematics, the closely related eutaxy condition precedes it by half a century. Voronoi's study [151] of quadratic forms in 1908 gave rise to the introduction of eutaxy condition (4.1.1). Nonetheless, we can say that a lattice is strongly eutactic whenever its set of minimal vectors forms a uniform tight frame. Another way to view uniform tight frames is as projective 1-designs, a subclass of more general designs on compact spaces introduced by Delsarte, Goethals, and Seidel in their groundbreaking 1977 paper [44]. A special class of tight frames are examples of optimal packings of lines in projective space, especiially those known as equiangular tight frames (ETFs). Tight frames in general and ETFs in particular are extensively studied objects in harmonic analysis; see S. Waldron's book [152] for detailed information on this subject.

Given a real (n, k)-frame $\mathcal{F} = \{\boldsymbol{f}_1, \dots, \boldsymbol{f}_n\}$, define

$$L(\mathcal{F}) = \operatorname{span}_{\mathbb{Z}} \{\boldsymbol{f}_1, \dots, \boldsymbol{f}_n\}.$$

If we write B for the $k \times n$ matrix with vectors $\boldsymbol{f}_1, \dots, \boldsymbol{f}_n$ as columns, then

$$L(\mathcal{F}) = \{B\boldsymbol{a} : \boldsymbol{a} \in \mathbb{Z}^n\}.$$

The *norm-form* associated with $\mathcal{F}$ is the quadratic form

$$Q_{\mathcal{F}}(\boldsymbol{a}) = \|B\boldsymbol{a}\|^2 = \langle B^\top B\boldsymbol{a}, \boldsymbol{a}\rangle. \tag{4.1.3}$$

We call the frame $\mathcal{F}$ *rational* if $Q_{\mathcal{F}}$ is (a constant multiple of) a rational quadratic form, i.e. the $n \times n$ Gram matrix $B^\top B$ is (a constant multiple of) a rational matrix. This is equivalent to saying that the inner products $\langle \boldsymbol{f}_i, \boldsymbol{f}_j \rangle$ are (up to a constant multiple) rational numbers for all $1 \leq i, j \leq n$. In [25], it was proved that if $\mathcal{F}$ is rational, then $L(\mathcal{F})$ is a lattice. Further, in the case that $\mathcal{F}$ is an ETF, $L(\mathcal{F})$ is a lattice if and only if $\mathcal{F}$ is rational (the converse was previously proved in [26]). More generally, it was shown in [25] that when the dimension $k = 2$ or 3 and $\mathcal{F}$ is a tight (n, k)-frame for any n so that $L(\mathcal{F})$ is a lattice, then $\mathcal{F}$ must be rational. Our first result is an extension of this observation to any dimension.

Theorem 4.1.1. Suppose that $\mathcal{F}$ is a tight (n, k)-frame so that $L(\mathcal{F})$ is a lattice. Then $\mathcal{F}$ must be rational.

We give two different proofs of Theorem 4.1.1 in Section 4.2, one of them as a consequence of a stronger result about a larger class of vector systems than tight frames (Theorem 4.2.3). All spherical 2-designs are tight frames, and a spherical 2-design when joined with its antipodes is additionally a spherical 3-design. We call a lattice L a *t-design lattice*, whenever L's minimal vectors form a t-design and L is generated by them. A classical result of Korkine and Zolotareff says that any t-design lattice with $t \geq 4$ is rational [83]. Our result extends this result showing that the same holds for t-design lattices with $t \geq 2$.

We found our Theorem 4.1.1 to appear earlier in the paper [140] (see Proposition 4.2 of [140]). This being said, our proof of this result is considerably simpler, and our Theorem 4.2.3 is more general: it does not follow from [140].

We may use this rationality result to pick out lattices generated by tight frames. We are especially interested in frames that give rise to lattices with nice geometric properties. For this we need some more notation. Let the automorphism group of a frame $\mathcal{F}$ be

$$\mathrm{Aut}(\mathcal{F}) := \{U \in \mathcal{O}_k(\mathbb{R}) : U\boldsymbol{f} \in \mathcal{F} \text{ for all } \boldsymbol{f} \in \mathcal{F}\},$$

where $\mathcal{O}_k(\mathbb{R})$ is the group of $k \times k$ real orthogonal matrices. As usual, we write $H \leq G$ to indicate that H is a subgroup of the group G.

We now discuss *group frames*; see Chapter 10 of [152] for a detailed exposition. Let $\boldsymbol{f}_1 \in \mathbb{R}^k$ be a vector and let G a finite group of orthogonal $k \times k$ matrices. Define $\mathcal{F}$ to be the orbit of $\boldsymbol{f}_1$ under the action of G by left multiplication, i.e.

$$\mathcal{F} = G\boldsymbol{f}_1 := \{U\boldsymbol{f}_1 : U \in G\},$$

then all the vectors in $\mathcal{F}$ have the same norm. If $\mathcal{F}$ spans $\mathbb{R}^k$, then $\mathcal{F}$ is a uniform frame, which we refer to as a G-*frame*. G is said to act *irreducibly* on the space $\mathbb{R}^k$ if there is no nonzero proper subspace E of $\mathbb{R}^k$ that is closed under the action of G, that is, $GE \neq E$ for any $\{\mathbf{0}\} \neq E \subsetneq \mathbb{R}^k$. A G-frame with such an irreducible action corresponding to G on $\mathbb{R}^k$ is similarly called irreducible. All irreducible group frames are tight. In fact, if G is a group with an irreducible action on $\mathbb{R}^k$, then the orbit of x under G, $\{U\boldsymbol{x} : U \in G\}$, is an irreducible tight G-frame for any nonzero vector $\boldsymbol{x} \in \mathbb{R}^k$ (see Sections 10.5 - 10.9 of [152] for details).

Our next result demonstrates a certain correspondence between irreducible group frames and strongly eutactic lattices.

Theorem 4.1.2. Let G be a group of $k \times k$ real orthogonal matrices and $\boldsymbol{f} \in \mathbb{R}^k$ be a vector so that

$\mathcal{F} = G\boldsymbol{f}$ is an irreducible rational group frame in $\mathbb{R}^k$. Then the lattice $L(\mathcal{F})$ is strongly eutactic.

Remark 4.1.3. Conversely, suppose $L \subset \mathbb{R}^k$ is a strongly eutactic lattice of rank k. By Corollary 16.1.3 of [103], L is strongly eutactic if and only if its set $S(L)$ of minimal vectors is a spherical 2-design, which is a condition equivalent to the tightness condition (4.1.2). Since all minimal vectors have the same norm, $S(L)$ is a uniform tight frame. Now suppose some $\mathrm{Aut}(L)$ acts transitively on $S(L)$. Let $\boldsymbol{x}_1 \in S(L)$, then for any $\boldsymbol{x} \in S(L)$ there exists a $U \in \mathrm{Aut}(L)$ such that $\boldsymbol{x} = U\boldsymbol{x}_1$. Hence

$$S(L) = \{U\boldsymbol{x}_1 : U \in \mathrm{Aut}(L)\},$$

and so $S(L)$ is an $\mathrm{Aut}(L)$-frame. If the action of $\mathrm{Aut}(L)$ on $\mathbb{R}^k$ is irreducible then $S(L)$ is an irreducible group frame.

We prove Theorem 4.1.2 in Section 4.3. This theorem motivates the investigation of rational irreducible group frames. One steady source of rational group frames comes from vertex transitive graphs, as detailed in Section 10.7 of [152]. In the special case when the graph in question is distance transitive, these frames are irreducible.

Theorem 4.1.4. Let Γ be a vertex transitive graph on n vertices and G its automorphism group. Let A be the adjacency matrix of Γ and λ an eigenvalue of multiplicity m. Assume λ is rational and let V_λ be the corresponding m-dimensional eigenspace to eigenvalue λ. Let P_λ be a rational orthogonal projection matrix of $\mathbb{R}^n$ onto V_λ. Then $L_{\Gamma,\lambda} := P_\lambda \mathbb{Z}^n$ is a lattice of full rank in V_λ, and its automorphism group contains a subgroup isomorphic to a factor group of G. If Γ is distance transitive, $L_{\Gamma,\lambda}$ is strongly eutactic.

We review all the necessary notation and prove Theorem 4.1.4 in Section 4.4. Distance transitive graphs form a subclass of vertex transitive graphs, and there are plenty of examples of such graphs with rational eigenvalues. In fact, there exist such lattices on n vertices for arbitrarily large n having eigenvalues of multiplicity m being an increasing function of n (for instance complete graphs, Johnson graphs, Grassman graphs, folded cube graphs, etc.), so that this construction yields plenty of strongly eutactic lattices. Further, there are some instances of vertex transitive graphs which

Graph Γ	Dist. trans.?	# of vert.	Eig. λ	Mult. of λ	Lattice $L_{\Gamma,\lambda}$
Disconnected graph	No	(n)	0	(n)	Integer lattice $\mathbb{Z}^n$
Complete graph K_n	Yes	(n)	-1	$(n-1)$	Root lattice A_{n-1}
Hamming graph $H(2,3)$	Yes	(9)	1	(4)	$A_2 \otimes_{\mathbb{Z}} A_2$
Petersen graph	Yes	(10)	-2	(4)	A_4^*, dual of A_4
Petersen graph	Yes	(10)	1	(5)	Coxeter lattice A_5^2
Petersen line graph	Yes	(15)	-1	(4)	A_4^*, dual of A_4
Petersen line graph	Yes	(15)	-2	(5)	Coxeter lattice A_5^3
Clebsch graph	Yes	(16)	-3	(5)	D_5^*, dual of D_5
Clebsch complement	Yes	(16)	2	(5)	D_5^*, dual of D_5
Shrikhande graph	No	(16)	2	(6)	D_6^+
Shrikhande complement	No	(16)	-3	(6)	D_6^+
Schläfli graph	Yes	(27)	4	(6)	E_6^*, dual of E_6
Schläfli complement	Yes	(27)	-5	(6)	E_6^*, dual of E_6
Gosset graph	Yes	(56)	9	(7)	E_7^*, dual of E_7

Table 4.1: Examples of strongly eutactic lattices from vertex transitive graphs

are not distance transitive, however still give rise to strongly eutactic lattices. We demonstrate several examples of our construction in Section 4.4, some of which are summarized in Table 4.1. A separate collection of lattices coming from several Johnson graphs $J(n,2)$ is given in Table 4.2 in Section 4.4. Furthermore, in Theorem 4.4.5 we give a characterization of lattices coming from product graphs in terms of tensor products and orthogonal direct sums of component lattices.

For the purposes of all of our examples and constructions, the lattices are viewed up to similarity and eigenspaces of graphs are identified with real Euclidean spaces $\mathbb{R}^k$ for the appropriate dimension k equal to the multiplicity of the corresponding eigenvalue. Our examples have been computed in Maple [100] using online catalog [5] of distance regular graphs and online catalog [102] of strongly eutactic lattices. It can be seen from these examples that a graph and its complement produce the same lattices. This is true in general, as is shown in Proposition 4.4.7 in Section 4.4. At the end of Section 4.4 we also demonstrate an interesting correspondence between contact polytopes of lattices E_6^*, E_7^* and A_3^* and our construction of lattices from their skeleton graphs.

Finally, in Section 4.5 we discuss a possible relation between coherence of a lattice and its sphere packing density, as well as potential applications of tight frames coming from sets of minimal vectors of lattices in compressed sensing.

4.2 Rationality of lattice-generating frames

We start with a simple proof of Theorem 4.1.1.

Proof of Theorem 4.1.1. With notation as in the statement of the theorem, let B be a $k \times n$ real matrix whose columns are vectors of the tight frame $\mathcal{F}$ and $L(\mathcal{F})$ is a lattice. Let A be a $k \times k$ basis matrix for $L(\mathcal{F})$. Then, there exists a $k \times n$ integer matrix Z so that $AZ = B$. Thus

$$AZZ^\top A^\top = BB^\top = \gamma I_k$$

for some $\gamma > 0$. Since A is invertible,

$$ZZ^\top = \gamma A^{-1}(A^\top)^{-1},$$

so that $ZZ^\top = \gamma(A^\top A)^{-1}$. Therefore

$$B^\top B = Z^\top A^\top AZ = Z^\top \gamma(ZZ^\top)^{-1}Z = \gamma Z^\top(ZZ^\top)^{-1}Z.$$

Since $Z^\top(ZZ^\top)^{-1}Z$ has rational entries, we have that $B^\top B$ is a multiple of a rational matrix. Therefore $\mathcal{F}$ is a rational tight frame. $\square$

The above argument implies that if $Q_{\mathcal{F}}$ as in (4.1.3) is a quadratic form corresponding to an irrational tight frame $\mathcal{F}$ then the corresponding integer span $L(\mathcal{F})$ is not a lattice (i.e. is not discrete) because $Q_{\mathcal{F}}$ cannot be bounded away from 0 on integer points. This argument, however, relies heavily on the norm-form $Q_{\mathcal{F}}$ coming from a tight frame. On the other hand, it is not difficult to construct other irrational quadratic forms (not corresponding to tight frames) which are bounded away from 0 on integer points. For instance, take $L_1, \dots, L_k$ to be rational linear forms in n variables

$x_1, \ldots, x_n$ and $c_1, \ldots, c_k$ any positive real numbers. Let

$$Q(x_1, ..., x_n) = c_1 L_1^2 + \cdots + c_k L_k^2.$$

This Q is a positive semidefinite quadratic form. Suppose $Q(\boldsymbol{a}) \neq 0$ for some integer vector $\boldsymbol{a}$, then there must exist $1 \leq i \leq k$ such that $L_i(a) \neq 0$. Since L_i has rational coefficients, $|L_i(a)| \geq 1/d_i$, where d_i is the least common multiple of the denominators of these coefficients. Let $d = \max\{d_1, \ldots, d_k\}$ and $c = \min\{c_1, \ldots, c_k\}$, then we have

$$Q(a) \geq c/d^2$$

for all $\boldsymbol{a}$ for which $Q(\boldsymbol{a}) \neq 0$. In particular, if some of the c_i's are irrational, Q is a form with irrational coefficients.

In view of this observation, it is interesting to understand what are the necessary and sufficient conditions on a $k \times n$ real matrix B so that $B\mathbb{Z}^n$ is a lattice to imply that B must be rational? In the rest of this section we prove a sufficient condition that is weaker than being a tight frame. Write $\{\boldsymbol{b}_i\}_{i=1}^n \subset \mathbb{R}^k$ for the elements of a frame $\mathcal{F}$ (a sequence of vectors spanning $\mathbb{R}^k$), written as column vectors of a $k \times n$ matrix B, where $n = k + m$. Let the first k columns in B be denoted in matrix form by B_0 and the remaining m column vectors by B_1, so that $B = [B_0 \mid B_1]$, $B_0 \in \mathbb{R}^{k \times k}$, $B_1 \in \mathbb{R}^{k \times m}$.

Lemma 4.2.1. Suppose that $B = [B_0 \mid B_1]$ is such that $B_0\mathbb{R}^k = \mathbb{R}^k$ and $\Lambda_B := B\mathbb{Z}^n$ is discrete. Then $B_0^{-1}B_1 \in \mathbb{Q}^{k \times m}$.

Proof. If Λ_B is discrete, it is a full-rank lattice in $\mathbb{R}^k$, and so has a basis matrix $A = \begin{pmatrix} \boldsymbol{a}_1 & \ldots & \boldsymbol{a}_k \end{pmatrix}$ such that $\Lambda_B = A\mathbb{Z}^k$. Hence there exist some integer matrices Z_0, Z_1 such that $AZ_0 = B_0$, and $AZ_1 = B_1$. Since B_0 is full rank and A invertible, Z_0 is invertible and $B_0^{-1}B_1 = Z_0^{-1}A^{-1}AZ_1 = Z_0^{-1}Z_1 \in \mathbb{Q}^{k \times m}$. $\square$

Let Q be an $k \times k$ orthogonal real matrix, then multiplication by Q preserves inner products of vectors in $\mathbb{R}^k$ and a collection of vectors $\{\boldsymbol{b}_i\}_{i=1}^n$ generates a lattice over $\mathbb{Z}$ if and only if $\{Q\boldsymbol{b}_i\}_{i=1}^n$ does. Let W be orthogonally equivalent to B, that is $W = QB$ for some $Q \in \mathcal{O}_k(\mathbb{R})$ ($\mathcal{O}_k(\mathbb{R})$ denotes the set of real $k \times k$ orthogonal matrices). $QQ^\top = I_k$, the $k \times k$ identity matrix, and the matrix of outer products for W is $WW^\top = QBB^\top Q^\top$. Having information about the entries of this matrix for certain Q (arising in this case from the QR-decomposition of a matrix) allows for an easy way to check rationality of inner products. When B is a tight frame given in matrix form, (as above) $BB^\top = \gamma I_k$ for some $\gamma > 0$, and so $WW^\top$ collapses to the same matrix as $BB^\top$. In general, however the relationship between $WW^\top$ and $BB^\top$ can get "muddled" by transformation so that determining lattice properties of integer combinations of vectors in a tight frame is easier than the general case.

Remark 4.2.2. Given $B_0 = QR$, the QR factorization of B_0, so that $Q \in \mathcal{O}_k(\mathbb{R})$ and R is upper-triangular with positive entries along the diagonal, it will be useful to work with the alternative representation of B: $\tilde{B} = Q^{-1}B = [R \mid Q^{-1}B_1]$.

In the arguments which follow, we choose to write $\tilde{B} = D[U \mid V]$, where $D \in \mathbb{R}^{k\times k}$ is diagonal with entries $d_1, ..., d_k$, $U \in \mathbb{R}^{k\times k}$ is upper-triangular with ones along the diagonal, and $V \in \mathbb{R}^{k\times m}$ is the remaining entries. In the above, d_i are taken to be positive (which is possible since R has positive diagonal entries). From now on, let B denote a matrix of the form $\tilde{B}$ when not specified otherwise.

Theorem 4.2.3. Suppose a collection of vectors $B = \{\boldsymbol{b}_i\}_{i=1}^n \subset \mathbb{R}^k$, $n = k+m$, is given as column vectors of a matrix of the form $\tilde{B}$ (as in the preceding remark). Suppose these column vectors have the following properties:

(i) $\operatorname{span}_{\mathbb{Z}} B$ is discrete,

(ii) the row-vectors of B, $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k$, satisfy $\langle \boldsymbol{r}_i, \boldsymbol{r}_j \rangle = d_i d_j q_{i,j}$ for some $q_{i,j} \in \mathbb{Q}$ and all $i \neq j$, that is, $[U \mid V][U \mid V]^T$ has rational entries off the diagonal, and

(iii) $\langle \boldsymbol{r}_i, \boldsymbol{r}_i \rangle = q_{i,i} \in \mathbb{Q}$ for all $i = 1, \ldots, k$, that is, $BB^T = D[U \mid V][U \mid V]^T D$ has rational entries on the diagonal.

$$\begin{pmatrix} d_1 & d_1u_{1,2} & d_1u_{1,3} & d_1u_{1,4} & \dots & d_1v_{1,1} & d_1v_{1,2} & \dots & d_1v_{1,m} \\ 0 & d_2 & d_2u_{2,3} & d_2u_{2,4} & \dots & d_2v_{2,1} & d_2v_{2,2} & \dots & d_2v_{2,m} \\ 0 & 0 & d_3 & d_3u_{3,4} & \dots & d_3v_{3,1} & d_3v_{3,2} & \dots & d_3v_{3,m} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & d_kv_{k,1} & d_kv_{k,2} & \dots & d_kv_{k,m} \end{pmatrix}$$

Figure 4.1: Matrix B obtained using QR factorization.

Then the inner products $\langle \boldsymbol{b}_i, \boldsymbol{b}_j \rangle$ must all be rational, i.e. $B^\top B \in \mathbb{Q}^{n\times n}$.

Proof. For each column vector $\boldsymbol{b}_j$ from B, Lemma 4.2.1 implies there exists a vector $\boldsymbol{p}_j \in \mathbb{Q}^k$ such that $B_0^{-1}\boldsymbol{b}_j = \boldsymbol{p}_j$. Letting $p_{i,j}$ be the i-th entry of each $\boldsymbol{p}_j$, we now use these rational numbers to demonstrate, under the above conditions, that $B^\top B$ must be rational.

Recall that B has k rows and $k+m$ columns. From now on, denote the last m column vectors of B by $\boldsymbol{v}_l$, $1 \le l \le m$. The condition $B_0^{-1}\boldsymbol{v}_l = \boldsymbol{p}_l$ gives that $d_kp_{k,l} = d_kv_{k,l}$, so $v_{k,l} = p_{k,l}$ for all $l = 1, \dots, m$, i.e., the numbers $v_{k,l}$ are rational. In the same manner, we obtain m equations:

$$d_{k-1}p_{k-1,l} + d_{k-1}u_{k-1,k}p_{k,l} = d_{k-1}v_{k-1,l},$$

which imply that $p_{k-1,l} + u_{k-1,k}p_{k,l} = v_{k-1,l}$ for all $l = 1, \dots, m$, as well as

$$d_kd_{k-1}(u_{k-1,k} + v_{k-1,1}v_{k,1} + \dots + v_{k-1,m}v_{k,m}) = q_{k,k-1}d_kd_{k-1},$$

which implies $u_{k-1,k} + v_{k-1,1}v_{k,1} + \dots + v_{k-1,m}v_{k,m} = q_{k,k-1}$. Now, these $m+1$ equations can be written together in a matrix equation:

$$\begin{pmatrix} 1 & v_{k,1} & v_{k,2} & \dots & v_{k,m} \\ p_{k,1} & -1 & 0 & \dots & 0 \\ p_{k,2} & 0 & -1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{k,m} & 0 & 0 & \dots & -1 \end{pmatrix} \begin{pmatrix} u_{k-1,k} \\ v_{k-1,1} \\ v_{k-1,2} \\ \vdots \\ v_{k-1,m} \end{pmatrix} = \begin{pmatrix} q_{k,k-1} \\ -p_{k-1,1} \\ -p_{k-1,2} \\ \vdots \\ -p_{k-1,m} \end{pmatrix}.$$

The matrix formed above on the left is invertible as all the rows of index greater than one are orthogonal to the first (this may be checked using the condition $v_{k,l} = p_{k,l}$) and the lower right block being the negative identity shows the last m rows (arising from the first set of equalities above) are linearly independent amongst themselves. Thus by applying the inverse of the matrix on the left to each side we can express the coordinates $u_{k-1,k}, v_{k-1,1}, \ldots, v_{k-1,m}$ of the vector on the left as rational numbers.

Proceeding, the idea now is to induct on "levels" (each level is determined by the smallest index in the variables appearing in the matrix equations of the type above) supposing that all the variables appearing in the previous level (with the exception of variables of the form d_i which must be treated separately later) have been demonstrated to be rational. At the i-th such level the arising matrix equation analogous to the one above is of the form:

$$\begin{pmatrix} 1 & u_{k-i+1,k-i+2} & u_{k-i+1,k-i+3} & \cdots & u_{k-i+1,k} & v_{k-i+1,1} & v_{k-i+1,2} & \cdots & v_{k-i+1,m} \\ 0 & 1 & u_{k-i+2,k-i+3} & \cdots & u_{k-i+2,k} & v_{k-i+2,1} & v_{k-i+2,2} & \cdots & v_{k-i+2,m} \\ 0 & 0 & 1 & \cdots & u_{k-i+3,k} & v_{k-i+3,1} & v_{k-i+3,2} & \cdots & v_{k-i+3,m} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & v_{k,1} & v_{k,2} & \cdots & v_{k,m} \\ p_{k-i+1,1} & p_{k-i+2,1} & p_{k-i+3,1} & \cdots & p_{k,1} & -1 & 0 & \cdots & 0 \\ p_{k-i+1,2} & p_{k-i+2,2} & p_{k-i+3,2} & \cdots & p_{k,2} & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{k-i+1,m} & p_{k-i+2,m} & p_{k-i+3,m} & \cdots & p_{k,m} & 0 & 0 & \cdots & -1 \end{pmatrix} \begin{pmatrix} u_{k-i,k-i+1} \\ u_{k-i,k-i+2} \\ u_{k-i,k-i+3} \\ \vdots \\ u_{k-i,k} \\ v_{k-i,1} \\ v_{k-i,2} \\ \vdots \\ v_{k-i,m} \end{pmatrix} = \begin{pmatrix} q_{k-i+1,k-i} \\ q_{k-i+2,k-i} \\ q_{k-i+3,k-i} \\ \vdots \\ q_{k,k-i} \\ -p_{k-i,1} \\ -p_{k-i,2} \\ \vdots \\ -p_{k-i,m} \end{pmatrix}.$$

As all entries in the matrix on the left appear in the left or right hand side vector of some matrix equation from a previous level, the inductive hypothesis implies that they are rational. A few observations are in order. The first i rows in the matrix above are linearly independent by the fact the first i column sub-matrix is upper-triangular with ones along the diagonal. Second, the remaining m row vectors have inner products with the first i row vectors which are zero as the expressions resulting in computing these inner products come exactly as the equations $B_0 \boldsymbol{p}_l = \boldsymbol{v}_l$.

Lastly, note that the last m row vectors are linearly independent amongst themselves by the lower right block being minus the identity in $\mathbb{R}^{m \times m}$. Together, these observations justify the claim that the above matrix is invertible, so that the variables $u_{k-i,k-i+1}, u_{k-i,k-i+2}, \ldots, u_{k-i,k}, v_{k-i,1}, \ldots, v_{k-i,m}$

may be expressed as rationals. This completes the inductive portion of the argument.

Reflect on what is known about the variables which have appeared in this process so far. For each i, the variables $\{u_{k-i,j+1}\}_{j=k-i}^{k-1}$ have been shown to be rational along with the variables $\{v_{k-i,j}\}_{j=1}^{m}$. There is one set of equations which have not appeared yet, along with a set of variables which have yet to play a role (the variables d_j). Treating these will be the last step of this argument.

The diagonal elements of $BB^\top$ give rise to the equations

$$d_l^2\left(1+\sum_{j=l}^{k-1}u_{l,j+1}^2+\sum_{i=1}^{m}v_{l,i}^2\right)=q_{l,l},\ l=1\ldots,k,$$

where the convention is that a sum with starting index larger than the ending index is zero. For $l=k$, the corresponding equation is

$$d_k^2\left(1+\sum_{i=1}^{m}v_{k,i}^2\right)=q_{k,k}.$$

Since all of the variables $v_{k,i}, q_{k,k}$ are rational, so is d_k^2. An analogous argument establishes that d_l^2 is rational as in those equations, $u_{l,j+1}, q_{l,l}$ and $v_{l,j}$ are rational (by the previous inductive argument). All that remains now is to compute the inner products. These are of the form

$$\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle=\sum_l d_l^2 v_{i,l}v_{j,l},\ \langle \boldsymbol{u}_i, \boldsymbol{u}_j\rangle=\sum_l d_l^2 u_{i,l+1}u_{j,l+1},\ \langle \boldsymbol{u}_i, \boldsymbol{v}_j\rangle=\sum_l d_l^2 u_{i,l+1}v_{j,l},$$

which are all rational. □

We now show that conditions of Theorem 4.2.3 include tight frames, thus providing an alternate proof of Theorem 4.1.1.

Corollary 4.2.4. Suppose that $B=\{\boldsymbol{b}_i\}_{i=1}^{n}\subset\mathbb{R}^k$ is a matrix with column vectors given by $\mathcal{F}$, a Parseval tight frame. Then $\operatorname{span}_{\mathbb{Z}}\mathcal{F}$ is discrete if and only if $\langle \boldsymbol{b}_i, \boldsymbol{b}_j\rangle$ are rational.

Proof. If the frame $\mathcal{F}$ is rational, then $\operatorname{span}_{\mathbb{Z}} \mathcal{F}$ is a lattice by Proposition 1 of [25]. The reverse implication follows by setting $q_{i,j} = 0$, $i \neq j$ and $q_{i,i} = 1$ in Theorem 4.2.3 (after computing the QR decomposition of B). $\square$

Second proof of Theorem 4.1.1. Suppose that $\mathcal{F} = \{\boldsymbol{f}_1, \dots, \boldsymbol{f}_n\}$ is a uniform tight (n,k)-frame so that $L(\mathcal{F}) = \operatorname{span}_{\mathbb{Z}} \mathcal{F}$ is a lattice. Then for all $\boldsymbol{v} \in \mathbb{R}^k$,

$$\|\boldsymbol{v}\|^2 = \gamma \sum_{i=1}^{n} \langle \boldsymbol{v}, \boldsymbol{f}_i \rangle^2 = \sum_{i=1}^{n} \langle \boldsymbol{v}, \sqrt{\gamma} \boldsymbol{f}_i \rangle^2$$

for an appropriate constant $\gamma > 0$. Hence $\mathcal{F}' = \sqrt{\gamma}\, \mathcal{F}$ is a Parseval tight frame and $\operatorname{span}_{\mathbb{Z}} \mathcal{F}' = \sqrt{\gamma}\, L(\mathcal{F})$ is again a lattice. Then Corollary 4.2.4 implies that inner products of vectors in $\mathcal{F}'$ are rational, and so inner products of vectors in $\mathcal{F}$ are rational multiples of $1/\gamma$. $\square$

4.3 Lattices from irreducible group frames

In this section we focus on group frames and lattices generated by them, in particular proving Theorem 4.1.2. As in Section 4.1, let $\boldsymbol{f}_1 \in \mathbb{R}^k$ be a vector and let G a finite group of orthogonal $k \times k$ matrices. Assume that

$$\mathcal{F} := \{U \boldsymbol{f}_1 : U \in G\},$$

spans $\mathbb{R}^k$, that is, it is a G-frame. If G is a cyclic group, $\mathcal{F}$ is called a *cyclic frame*. An example of a cyclic frame is the $(k, k+1)$-ETF discussed, for instance, in Section 5 of [26]:

$$f_1 = \frac{1}{\sqrt{k^2+k}} \begin{pmatrix} -k \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \dots, f_{k+1} = \frac{1}{\sqrt{k^2+k}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ -k \end{pmatrix}. \tag{4.3.1}$$

If G is an abelian group, $\mathcal{F}$ is a *harmonic frame* (see Section 11.3 of [152], Theorem 11.1). Notice that for any G-frame $\mathcal{F}$, $G \leq \operatorname{Aut}(\mathcal{F})$. We also make a simple observation about the size of the

G-frame $\mathcal{F}$.

Lemma 4.3.1. Let $\mathcal{F} := \{U\boldsymbol{f}_1 : U \in G\}$ be a G-frame in $\mathbb{R}^k$, then $|\mathcal{F}|= |G : G_{\boldsymbol{f}_1}|$ where $G_{\boldsymbol{f}_1}$ is the stabilizer of $\boldsymbol{f}_1$ and $|\mathcal{F}|\leq |G|$. Further, $|\mathcal{F}|< |G|$ if and only if $\boldsymbol{f}_1$ is an eigenvector for some non-identity matrix $W \in G$ with the corresponding eigenvalue equal to 1.

Proof. The fact that $|\mathcal{F}|= |G : G_{\boldsymbol{f}_1}|\leq |G|$ is clear from the definition. Now assume $|\mathcal{F}|< |G|$, which is equivalent to saying that $|G_{\boldsymbol{f}_1}|> 1$. This is true if and only if there exists a non-identity matrix $W \in G$ such that $W\boldsymbol{f}_1 = \boldsymbol{f}_1$. □

Proof of Theorem 4.1.2. The automorphism group of $L(\mathcal{F})$, $\mathrm{Aut}(L(\mathcal{F}))$, is the group of all orthogonal matrices that permute the lattice. Then we have

$$G \leq \mathrm{Aut}(\mathcal{F}) \leq \mathrm{Aut}(L(\mathcal{F})),$$

and the action of G on $\mathbb{R}^k$ is irreducible. Let $S(L(\mathcal{F}))$ be the set of minimal vectors of $L(\mathcal{F})$ and let $E = \mathrm{span}_{\mathbb{R}} S(L(\mathcal{F}))$. Since the automorphisms of $L(\mathcal{F})$ permute the minimal vectors, it must be true that E is closed under the action of G. Thus we must have $E = \mathbb{R}^k$, and so G acts irreducibly on E, the space spanned by the minimal vectors of $L(\mathcal{F})$. Then Theorem 3.6.6 of [103] guarantees that $S(L(\mathcal{F}))$ is a strongly eutactic configuration, and hence $L(\mathcal{F})$ is a strongly eutactic lattice. □

4.4 Vertex transitive graphs

Construction of group frames from vertex transitive graphs is described in Section 10.7 of [152]. We briefly review this subject here, proving Theorem 4.1.4 and providing some applications.

Let Γ be a graph on n vertices labeled by integers $1, \dots, n$ with automorphism group $G := \mathrm{Aut}(\Gamma)$. Γ is called *vertex transitive* if for each pair of vertices i, j there exists $\tau \in G$ such that $\tau(i) = j$. We define the *distance* between two vertices in a graph to be the number of edges in a shortest path connecting them. A connected graph Γ is called *distance transitive* if for any two pairs of vertices i, j and k, l at the same distance from each other there existence an automorphism $\tau \in G$

such that $\tau(i) = k$ and $\tau(j) = l$. Clearly, distance transitive graphs are always vertex transitive, but the converse is not true. From here on graphs considered will always be vertex transitive, and we will indicate specifically when we need them to also be distance transitive. Let $\boldsymbol{e}_1, \dots, \boldsymbol{e}_n$ denote the standard basis vectors in $\mathbb{R}^n$. Then G acts on $\mathbb{R}^n$ by

$$\tau\left(\sum_{i=1}^{n} c_i \boldsymbol{e}_i\right) = \sum_{i=1}^{n} c_i \boldsymbol{e}_{\tau(i)}$$

for every $\tau \in G$ and vector $\sum_{i=1}^n c_i \boldsymbol{e}_i \in \mathbb{R}^n$. Let $A = (a_{ij})$ be the $n \times n$ adjacency matrix of Γ, so that $a_{ij} = 1$ if vertices i and j are connected by an edge and $a_{ij} = 0$ otherwise. Then $a_{\tau(i)\tau(j)} = a_{ij}$ for all $\tau \in G$. The matrix A is symmetric, with real eigenvalues $\lambda_1, \dots, \lambda_k$, each of multiplicity m_{λ_i}, so that $\sum_{i=1}^k m_{\lambda_i} = n$. From now on, we call these the eigenvalues of the graph Γ. For each λ_i let $V_{\lambda_i} \subset \mathbb{R}^n$ be the corresponding m_{λ_i}-dimensional eigenspace. The group G acts on each eigenspace V_{λ_i} and for any nonzero vector $\boldsymbol{v} \in V_{\lambda_i}$ the orbit $G\boldsymbol{v}$ of $\boldsymbol{v}$ under the action of G is a group frame in $V_{\lambda_i} \cong \mathbb{R}^{m_i}$. When Γ is a distance transitive graph, this action of G on V_{λ_i} is irreducible, hence producing an irreducible group frame (see Proposition 4.1.11 on p. 137 of [23]). Further, if P_{λ_i} is the orthogonal projection onto V_{λ_i}, then for any $\tau \in G$ and $\boldsymbol{x} \in \mathbb{R}^n$,

$$\tau(P_{\lambda_i}(\boldsymbol{x})) = P_{\lambda_i}(\tau(\boldsymbol{x})).$$

As indicated in Section 10.7 of [152], this identity is true since the action of $\tau \in G$ and the action of the adjacency matrix A on a vector commute, i.e.

$$\tau(A\boldsymbol{e}_k) = \sum_i a_{ik} \tau \boldsymbol{e}_i = \sum_j a_{\tau^{-1}(j),k} \boldsymbol{e}_j = \sum_j a_{j,\tau(k)} \boldsymbol{e}_j = A(\tau(\boldsymbol{e}_k)).$$

Proof of Theorem 4.1.4. Suppose now that an eigenvalue λ_i is an integer. We know that the group G consists of permutation matrices. Pick a nonzero integer vector $\boldsymbol{x} \in \mathbb{R}^n$. Then $P_{\lambda_i}\boldsymbol{x} \in V_{\lambda_i}$ and the frame $\mathcal{F}_{\lambda_i}(\boldsymbol{x}) := GP_{\lambda_i}\boldsymbol{x} = P_{\lambda_i}(G\boldsymbol{x})$ is rational, and hence generates a lattice $L(\mathcal{F}_{\lambda_i}(\boldsymbol{x})) = \operatorname{span}_{\mathbb{Z}} \mathcal{F}_{\lambda_i}(\boldsymbol{x})$. This lattice is strongly eutactic if this group frame is irreducible, which is the case when the graph is distance transitive. Let H be the kernel of the action of G on V_{λ_i}, i.e.

$$H = \{\tau \in G : \tau(\boldsymbol{x}) = \boldsymbol{x} \text{ for all } \boldsymbol{x} \in V_{\lambda_i}\}.$$

Notice that H is a normal subgroup of G, since for any $\sigma \in G$ and $\boldsymbol{x} \in V_{\lambda_i}$, $\sigma(\boldsymbol{x}) \in V_{\lambda_i}$, and so

$$(\tau\sigma)(\boldsymbol{x}) = \tau(\sigma(\boldsymbol{x})) = \sigma(\boldsymbol{x}) = \sigma(\tau(\boldsymbol{x})) = (\sigma\tau)(\boldsymbol{x}),$$

for any $\tau \in H$. Then the quotient group G/H is isomorphic to a subgroup of $\mathrm{Aut}(L(\mathcal{F}_{\lambda_i}))$. If $\boldsymbol{x} = \boldsymbol{e}_1$, then the corresponding frame

$$\mathcal{F}_{\lambda_i} := \mathcal{F}_{\lambda_i}(\boldsymbol{e}_1)$$

consists of column vectors of P_{λ_i} (possibly with repetitions), since $\tau\boldsymbol{e}_1$ is some $\boldsymbol{e}_j$ for every $\tau \in G$, and every $\boldsymbol{e}_j$ is representable as $\tau\boldsymbol{e}_1$ for some $\tau \in G$, since the graph is vertex transitive. Then the resulting lattice $L(\mathcal{F}_{\lambda_i}) = P_{\lambda_i}\mathbb{Z}^n$, and this concludes the proof of Theorem 4.1.4. $\square$

We refer to the lattice $L(\mathcal{F}_{\lambda_i})$ described above as lattice *generated* by the graph Γ and denote it by L_{Γ,λ_i}.

Remark 4.4.1. While our proof that the lattice L_{Γ,λ_i} is strongly eutactic only applies to the situations when Γ is distance transitive, there are examples of vertex transitive graphs which are not distance transitive that nonetheless still produce strongly eutactic lattices: we demonstrate some such examples below. It would be interesting to understand if this is indeed the case for all vertex transitive graphs, or if there exist some that generate lattices that are not strongly eutactic.

For the rest of this section, we consider examples of this lattice construction when applied to various graphs and their products. One class of lattices that will figure prominently in our examples are *root lattices*, that is, integral lattices generated by vectors of norm 2, which are called its *roots* (recall that a lattice is integral if the inner product between any two vectors is always an integer).

Also recall that the *dual lattice* of a full rank lattice $L \subset \mathbb{R}^n$ is

$$L^* := \{\boldsymbol{x} \in \mathbb{R}^n : \langle \boldsymbol{x}, \boldsymbol{y} \rangle \in \mathbb{Z} \text{ for all } \boldsymbol{y} \in L\}.$$

If L is integral, then $L \subseteq L^*$.

Lemma 4.4.2. Let 0_n be a completely disconnected graph on n vertices, then 0_n generates the integer lattice $\mathbb{Z}^n$.

Proof. The adjacency matrix for 0_n is the $n \times n$ 0-matrix, and so it has one eigenvalue 0 with multiplicity n with the corresponding eigenspace being the entire $\mathbb{R}^n$. The automorphism group of 0_n is S_n, so the group frame obtained from the vector $\boldsymbol{e}_1$ is the full standard basis, which spans the lattice $\mathbb{Z}^n$. □

Lemma 4.4.3. The complete graph K_n generates (a lattice similar to) the root lattice

$$A_{n-1} = \left\{ \boldsymbol{x} \in \mathbb{Z}^n : \sum_{i=1}^{n} x_i = 0 \right\}.$$

Proof. The complete graph K_n is the graph on n vertices with no loops in which every vertex is connected to every other. Hence adjacency matrix A has 1's for all the off-diagonal entries and 0's on the diagonal. There are two eigenvalues: $\lambda_1 = -1$ with multiplicity $n-1$ and $\lambda_2 = n-1$ with multiplicity 1. The eigenspace corresponding to λ_2 is $V_{n-1} = \operatorname{span}_{\mathbb{R}}\{(1,\dots,1)^\top\}$ and the eigenspace V_{-1} corresponding to λ_1 is the orthogonal complement of V_{n-1} in $\mathbb{R}^n$. The automorphism group of K_n is S_n. The orthogonal projection onto V_{-1} is given by

$$P_{-1} = \frac{1}{n-1} \begin{pmatrix} n-1 & -1 & \dots & -1 \\ -1 & n-1 & \dots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \dots & n-1 \end{pmatrix},$$

so the lattice $L_{K_n,-1}$ generated by the columns of P_{-1} is the root lattice $A_{n-1} = \mathbb{Z}^n \cap V_{-1}$ rescaled by the factor $1/(n-1)$. $\square$

Next we consider graphs that are constructed as products of smaller graphs. We start with disjoint unions. In order for such a graph to be vertex transitive, all the components in the disjoint union need to be vertex transitive and isomorphic to each other. Hence we can think of them as copies of the same vertex transitive graph.

Lemma 4.4.4. Let Γ be a vertex transitive graph constructed as a disjoint union of k copies of a vertex transitive graph Δ. Let λ be a rational eigenvalue of Δ and $L_{\Delta,\lambda}$ be a lattice generated by the λ-eigenspace of Δ. Then Γ also has λ as an eigenvalue and generates a lattice given by the orthogonal sum of k copies of $L_{\Delta,\lambda}$.

Proof. Let m be the number of vertices of Δ and let A_Δ be its adjacency matrix. Then the $mk \times mk$ adjacency matrix A_Γ of the graph Γ is a block matrix with diagonal $m \times m$ blocks being A_Δ and the rest filled up with 0 blocks, i.e.

$$A_\Gamma = \begin{pmatrix} A_\Delta & 0 & \dots & 0 \\ 0 & A_\Delta & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & A_\Delta \end{pmatrix}.$$

Let us refer to a block matrix like this as $\bigoplus_k(A_\Delta)$. A_Γ has the same eigenvalues as A_Δ, but of k times greater multiplicity. Let $V_{\Delta,\lambda}$ be the λ-eigenspace of A_Δ with the corresponding projection matrix $P_{\Delta,\lambda}$. The λ-eigenspace of A_Γ is the orthogonal sum of k copies of $V_{\Delta,\lambda}$ and the corresponding projection matrix is $\bigoplus_k(P_{\Delta,\lambda})$. Hence the lattice $L_{\Gamma,\lambda}$ generated by the column vectors of this matrix is the orthogonal sum of k copies of $L_{\Delta,\lambda}$. $\square$

Now we recall the three fundamental commutative product constructions of graphs (see [70] and [75] for detailed information). In each of these constructions, each eigenvalue ν of the product graph Γ is derived from a pair of eigenvalues λ and μ of the component graphs Δ_1 and Δ_2, respectively, via some function $f(\lambda, \mu)$. This function f differs depending on which product we consider. Spectral properties of product graphs are nicely summarized in [127].

The *Cartesian product* of two graphs Δ_1 and Δ_2, denoted $\Delta_1 \Box \Delta_2$, is the graph whose vertices are pairs (u, v), where u is a vertex of Δ_1 and v is a vertex of Δ_2, and two vertices (u_1, v_1) and (u_2, v_2) are connected by an edge if and only if either $u_1 = u_2$ and v_1, v_2 are connected by an edge in Δ_2, or $v_1 = v_2$ and u_1, u_2 are connected by an edge in Δ_1. Then $\Delta_1 \Box \Delta_2$ is vertex transitive if and only if both Δ_1 and Δ_2 are vertex transitive ([66], Section 7.14, or [70]). For each pair of eigenvalues λ of Δ_1 and μ of Δ_2, there is an eigenvalue ν of $\Delta_1 \Box \Delta_2$ given by

$$\nu = f(\lambda, \mu) := \lambda + \mu,$$

and if $\boldsymbol{u}, \boldsymbol{v}$ are corresponding eigenvectors of Δ_1, Δ_2, respectively, then $\boldsymbol{u} \otimes \boldsymbol{v}$ is an eigenvector of Γ corresponding to ν.

The *direct product* of two graphs Δ_1 and Δ_2, denoted $\Delta_1 \times \Delta_2$ is the graph whose vertices are pairs (u, v), where u is a vertex of Δ_1 and v is a vertex of Δ_2, and two vertices (u_1, v_1) and (u_2, v_2) are connected by an edge if and only if both pairs u_1, u_2 and v_1, v_2 are connected by an edge in Δ_1, Δ_2, respectively. If Δ_1 and Δ_2 are vertex transitive, then $\Delta_1 \times \Delta_2$ is vertex transitive. The converse statement is not as straight-forward, and distinguishes between bipartite and non-bipartite graphs (see [69]). For each pair of eigenvalues λ of Δ_1 and μ of Δ_2, there is an eigenvalue ν of $\Delta_1 \times \Delta_2$ given by

$$\nu = f(\lambda, \mu) := \lambda\mu,$$

and if $\boldsymbol{u}, \boldsymbol{v}$ are corresponding eigenvectors of Δ_1, Δ_2, respectively, then $\boldsymbol{u} \otimes \boldsymbol{v}$ is an eigenvector of Γ corresponding to ν.

The *strong product* of two graphs Δ_1 and Δ_2, denoted $\Delta_1 \boxtimes \Delta_2$, is the graph whose vertices are pairs (u, v), where u is a vertex of Δ_1 and v is a vertex of Δ_2, and two vertices (u_1, v_1) and (u_2, v_2) are connected by an edge if and only if u_1, u_2 and v_1, v_2 are either equal or connected by an edge in Δ_1, Δ_2, respectively. The graph $\Delta_1 \boxtimes \Delta_2$ is vertex transitive if and only if both Δ_1 and Δ_2 are vertex transitive (Section 7.4 of [70]). For each pair of eigenvalues λ of Δ_1 and μ of Δ_2, there is an eigenvalue ν of $\Delta_1 \boxtimes \Delta_2$ given by

$$\nu = f(\lambda, \mu) := (\lambda + 1)(\mu + 1) - 1,$$

and if $\boldsymbol{u}, \boldsymbol{v}$ are corresponding eigenvectors of Δ_1, Δ_2, respectively, then $\boldsymbol{u} \otimes \boldsymbol{v}$ is an eigenvector of Γ corresponding to ν.

The *lexicographic product* of two vertex transitive graphs Δ_1 and Δ_2 is a vertex transitive graph whose vertices are pairs (u, v), where u is a vertex of Δ_1 and v is a vertex of Δ_2, and two vertices (u_1, v_1) and (u_2, v_2) are connected by an edge if and only if either u_1, u_2 are connected in Δ_1, or $u_1 = u_2$ and v_1, v_2 are connected in Δ_2.

For two vectors $\boldsymbol{x} \in \mathbb{R}^{m_1}, \boldsymbol{y} \in \mathbb{R}^{m_2}$ and $m_1 \times m_1$, $m_2 \times m_2$ matrices A, B, respectively, we have

$$(A\boldsymbol{x}) \otimes (B\boldsymbol{y}) = (A \otimes B)(\boldsymbol{x} \otimes \boldsymbol{y}), \tag{4.4.1}$$

where $\otimes$ stands for the usual Kronecker (outer) product of matrices and vectors. Further, if two vectors $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^{m_1}$ are orthogonal and $\boldsymbol{y} \in \mathbb{R}^{m_2}$, then simple tensors $\boldsymbol{x}_1 \otimes \boldsymbol{y}$ and $\boldsymbol{x}_2 \otimes \boldsymbol{y}$ are also orthogonal.

Theorem 4.4.5. Let Δ_1, Δ_2 be vertex transitive graphs on m_1, m_2 vertices, respectively, and let Γ be a product graph

$$\Gamma = \Delta_1 * \Delta_2$$

on $m_1 m_2$ vertices, where $*$ stands for $\square$, $\times$, or $\boxtimes$. Let ν be an eigenvalue of Γ and (λ_i, μ_i) for $1 \leq i \leq k$ pairs of eigenvalues of Δ_1, Δ_2 respectively so that

$$\nu = f(\lambda_i, \mu_i) \text{ for all } 1 \leq i \leq k$$

for the appropriate f. Let L_{Δ_1, λ_i} and L_{Δ_2, μ_i} for each $1 \leq i \leq k$ be the corresponding lattices. Then

$L_{\Gamma,\nu}$ is the orthogonal projection of $\mathbb{Z}^{m_1 m_2}$ onto the space spanned by

$$(L_{\Delta_1,\lambda_1} \otimes_{\mathbb{Z}} L_{\Delta_2,\mu_1}) \oplus \cdots \oplus (L_{\Delta_1,\lambda_k} \otimes_{\mathbb{Z}} L_{\Delta_2,\mu_k}),$$

where $\oplus$ is the orthogonal direct sum. In particular, if $k = 1$ then

$$L_{\Gamma,\nu} = L_{\Delta_1,\lambda_1} \otimes_{\mathbb{Z}} L_{\Delta_2,\mu_1},$$

up to similarity.

Proof. Let V_{Δ_1,λ_i}, W_{Δ_2,μ_i} be the eigenspaces of Δ_1, Δ_2 corresponding to λ_i, μ_i, respectively, with the corresponding orthogonal projection matrices P_{Δ_1,λ_i}, P_{Δ_2,μ_i}. Then

$$L_{\Delta_1,\lambda_i} = P_{\Delta_1,\lambda_i}\mathbb{Z}^{m_1} \subset V_{\Delta_1,\lambda_i},\ L_{\Delta_2,\mu_i} = P_{\Delta_2,\mu_i}\mathbb{Z}^{m_2} \subset W_{\Delta_2,\mu_i},$$

and $V_{\Delta_1,\lambda_i} = \operatorname{span}_{\mathbb{R}} L_{\Delta_1,\lambda_i}$, $W_{\Delta_2,\mu_i} = \operatorname{span}_{\mathbb{R}} L_{\Delta_2,\mu_i}$, so

$$V_{\Delta_1,\lambda_i} \otimes_{\mathbb{R}} W_{\Delta_2,\mu_i} = \operatorname{span}_{\mathbb{R}} (L_{\Delta_1,\lambda_i} \otimes_{\mathbb{Z}} L_{\Delta_2,\mu_i}).$$

Since adjacency matrices of graphs are symmetric, the eigenspaces corresponding to distinct eigenvalues are orthogonal, so that any two V_{Δ_1,λ_i} are orthogonal to each other, as are any two W_{Δ_2,μ_i}. Then each two $V_{\Delta_1,\lambda_i} \otimes_{\mathbb{R}} W_{\Delta_2,\mu_i}$ are also orthogonal to each other, and the eigenspace of Γ corresponding to ν is

$$\begin{aligned} U_{\Gamma,\nu} = P_{\Gamma,\nu}\mathbb{R}^{m_1 m_2} &= (P_{\Delta_1,\lambda_1} \otimes P_{\Delta_2,\mu_1})\mathbb{R}^{m_1 m_2} \oplus \cdots \oplus (P_{\Delta_1,\lambda_k} \otimes P_{\Delta_2,\mu_k})\mathbb{R}^{m_1 m_2} \\ &= (P_{\Delta_1,\lambda_1}\mathbb{R}^{m_1} \otimes_{\mathbb{R}} P_{\Delta_2,\mu_1}\mathbb{R}^{m_2}) \oplus \cdots \oplus (P_{\Delta_1,\lambda_k}\mathbb{R}^{m_1} \otimes_{\mathbb{R}} P_{\Delta_2,\mu_k}\mathbb{R}^{m_2}) \\ &= (V_{\Delta_1,\lambda_1} \otimes_{\mathbb{R}} W_{\Delta_2,\mu_1}) \oplus \cdots \oplus (V_{\Delta_1,\lambda_k} \otimes_{\mathbb{R}} W_{\Delta_2,\mu_k}), \end{aligned}$$

by (4.4.1), where $P_{\Gamma,\nu}$ is the orthogonal projection matrix onto $U_{\Gamma,\nu}$; we are using here the fact that

$\mathbb{R}^{m_1} \otimes_{\mathbb{R}} \mathbb{R}^{m_2} = \mathbb{R}^{m_1 m_2}$. Then $L_{\Gamma,\nu} = P_{\Gamma,\nu}\mathbb{Z}^{m_1 m_2}$.

Now suppose $k = 1$, then applying (4.4.1) again and using that $\mathbb{Z}^{m_1} \otimes_{\mathbb{Z}} \mathbb{Z}^{m_2} = \mathbb{Z}^{m_1 m_2}$, we have:

$$L_{\Gamma,\nu} = P_{\Gamma,\nu}\mathbb{Z}^{m_1 m_2} = (P_{\Delta_1,\lambda_1} \otimes P_{\Delta_2,\mu_1})\,\mathbb{Z}^{m_1 m_2} = P_{\Delta_1,\lambda_1}\mathbb{Z}^{m_1} \otimes_{\mathbb{Z}} P_{\Delta_2,\mu_1}\mathbb{Z}^{m_2} = L_{\Delta_1,\lambda_1} \otimes_{\mathbb{Z}} L_{\Delta_2,\mu_1}.$$

This completes the proof. $\square$

Example 4.4.6. Let Δ_1 be the complete graph K_3 and Δ_2 the 4-cycle graph C_4. Eigenvalues of K_3 are $\lambda_1 = 2$ (multiplicity 1) and $\lambda_2 = -1$ (multiplicity 2); eigenvalues of C_4 are $\mu_1 = 2$ (multiplicity 1), $\mu_2 = -2$ (multiplicity 1), $\mu_3 = 0$ (multiplicity 2). The corresponding lattices are

$$L_{K_3,2} = \frac{1}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\mathbb{Z},\ L_{K_3,-1} = \frac{1}{3}\begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix}\mathbb{Z}^2,$$

and

$$L_{C_4,2} = \frac{1}{4}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}\mathbb{Z},\ L_{C_4,-2} = \frac{1}{4}\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}\mathbb{Z},\ L_{C_4,0} = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}\mathbb{Z}^2.$$

Let $\Gamma_1 = K_3 \square C_4$, then $\nu = -1$ is an eigenvalue of Γ_1, obtained in a unique way as $\nu = \lambda_2 + \mu_3$, hence

$$L_{\Gamma_1,-1} = L_{K_3,-1} \otimes_{\mathbb{Z}} L_{C_4,0} \sim A_2 \otimes_{\mathbb{Z}} \mathbb{Z}^2 = A_2 \oplus A_2.$$

Let $\Gamma_2 = K_3 \times C_4$, then $\nu = 0$ is an eigenvalue of Γ_2, obtained as

$$\nu = \lambda_1\mu_3 = \lambda_2\mu_3,$$

hence $L_{\Gamma_2,0}$ is the orthogonal projection of $\mathbb{Z}^{12}$ onto the space spanned by

$$(L_{K_3,2} \otimes_{\mathbb{Z}} L_{C_4,0}) \oplus (L_{K_3,-1} \otimes_{\mathbb{Z}} L_{C_4,0}) = (L_{K_3,2} \oplus L_{K_3,-1}) \otimes_{\mathbb{Z}} L_{C_4,0} \sim \mathbb{Z}^3 \otimes_{\mathbb{Z}} \mathbb{Z}^2 = \mathbb{Z}^6.$$

Hence $L_{\Gamma_2,0}$ is similar to $\mathbb{Z}^6$.

Let $\Gamma_3 = K_3 \boxtimes C_4$, then $\nu = -1$ is an eigenvalue of Γ_2, obtained as

$$\nu = (\lambda_1 + 1)(\mu_1 + 1) - 1 = (\lambda_1 + 1)(\mu_2 + 1) - 1 = (\lambda_1 + 1)(\mu_3 + 1) - 1,$$

hence $L_{\Gamma_3,-1}$ is the orthogonal projection of $\mathbb{Z}^{12}$ onto the space spanned by

$$\begin{aligned} & (L_{K_3,-1} \otimes_{\mathbb{Z}} L_{C_4,2}) \oplus (L_{K_3,-1} \otimes_{\mathbb{Z}} L_{C_4,-2}) \oplus (L_{K_3,-1} \otimes_{\mathbb{Z}} L_{C_4,0}) \\ = \; & L_{K_3,-1} \otimes_{\mathbb{Z}} (L_{C_4,2} \oplus L_{C_4,-2} \oplus L_{C_4,0}) \sim A_2 \otimes_{\mathbb{Z}} \mathbb{Z}^4 \\ = \; & A_2 \oplus A_2 \oplus A_2 \oplus A_2. \end{aligned}$$

Hence $L_{\Gamma_2,0}$ is similar to $A_2 \oplus A_2 \oplus A_2 \oplus A_2$.

Let $\Gamma_4 = K_3 \circ C_4$ be the lexicographic product of K_3 by C_4. Unlike the previously considered products, this one is not commutative.Then eigenvalues of Γ_4 are 10 (multiplicity 1), 0 (multiplicity 6), -2 (multiplicity 5). The lattice $L_{\Gamma_4,-2}$ is similar to A_5^*, and the lattice $L_{\Gamma_4,0}$ is similar to $\mathbb{Z}^6$.

We also discuss a relation between lattices generated by a graph and by its complement. If Γ is a graph on n vertices, then its complement Γ' is a graph on the same vertices that has no common edges with Γ and so when 'put together' the two form a complete graph K_n. Vertex transitive graphs are regular, so let k be the common degree of the vertices of Γ. Then $n - k - 1$ is the common degree of the vertices of Γ'. So k is an eigenvalue of Γ of multiplicity 1 with the corresponding eigenvector $\mathbf{1} := (1, \ldots, 1)^\top$ and $n - k - 1$ is an eigenvalue of Γ' of the same multiplicity with the same corresponding eigenvector. Moreover the following result holds.

Proposition 4.4.7. Let Γ be a vertex transitive graph on n vertices of degree k and Γ' its complement.

Then for each eigenvalue $\lambda \neq k$ of Γ there is an eigenvalue $\lambda' = -\lambda - 1$ of Γ' of the same multiplicity and the lattices $L_{\Gamma,\lambda}$ and $L_{\Gamma',\lambda'}$ are the same.

Proof. It is well known that if $p(x)$ is the characteristic polynomial of the adjacency matrix A of Γ, then the characteristic polynomial of the adjacency matrix B of Γ' is

$$q(x) = (-1)^n \frac{x - n + k + 1}{x + k + 1} p(-x - 1),$$

and so for each eigenvalue $\lambda \neq k$ of Γ there is an eigenvalue $\lambda' = -\lambda - 1$ of Γ' of the same multiplicity (see, for instance, p. 27 of [22]). Further, the adjacency matrices satisfy the relation

$$B = J_n - I_n - A,$$

where I_n is the $n \times n$ identity matrix and J_n is the $n \times n$ matrix consisting of all 1's. Let $\lambda \neq k$ be an eigenvalue of Γ with a corresponding eigenvector $\boldsymbol{x}$. Since eigenspaces of Γ corresponding to different eigenvalues are orthogonal, $\boldsymbol{x}$ must be orthogonal to $\mathbf{1}$, which means that

$$\sum_{i=1}^{n} x_i = 0,$$

and so $J_n \boldsymbol{x} = \mathbf{0}$. Then

$$B\boldsymbol{x} = J_n \boldsymbol{x} - \boldsymbol{x} - \lambda \boldsymbol{x} = (-\lambda - 1)\boldsymbol{x},$$

i.e. $\boldsymbol{x}$ is an eigenvector of B corresponding to the eigenvalue λ'. This means that the eigenspace of Γ' corresponding to the eigenvalue $\lambda' = -\lambda - 1$ is the same as the eigenspace of Γ corresponding to the eigenvalue λ, hence they generate the same lattices. $\square$

We now consider more examples. In all the examples to follow, lattices are specified up to similarity. Information about the graphs we mention can be found, for instance, in [22].

Example 4.4.8. Recall the construction of the Hamming graph $H(d, q)$: if S is a set of q elements and d a positive integer, then vertex set of $H(d, q)$ is S^d, the set of ordered d-tuples of elements of S, and two vertices are connected by an edge if they differ in precisely one coordinate. $H(d,q)$ has eigenvalues $(q-1)d - qi$ with multiplicity $\binom{d}{i}(q-1)^i$ for $0 \leq i \leq d$. It is well known that $H(d,q)$ is the Cartesian product of d complete graphs K_q, and hence gives rise to product lattices. Hamming graphs are known to be distance transitive.

For instance, $H(2,3)$ has 9 vertices and three eigenvalues: 4 (multiplicity 1), -2 (multiplicity 4) and 1 (multiplicity 4). Projection matrices of both of the 4-dimensional eigenspaces give rise to the same tensor product lattice: $A_2 \otimes_{\mathbb{Z}} A_2$.

On the other hand, the graph $H(3,2)$ has 8 vertices and is isomorphic to the cube graph Q_3, i.e.

$$H(3,2) = K_2 \Box K_2 \Box K_2 = K_2 \Box C_4,$$

where C_4 is as in Example 4.4.6 with eigenvalues μ_1, μ_2, μ_3 and the corresponding lattices, and K_2 that has multiplicity 1 eigenvalues $\lambda_1 = 1$, $\lambda_2 = -1$ with

$$L_{K_2,1} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\mathbb{Z},\ L_{K_2,-1} = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\mathbb{Z}.$$

Therefore eigenvalues of $H(3,2)$ are:

- 1 (multiplicity 3), obtained in 2 ways: $\lambda_1 + \mu_3 = 1 + 0$ and $\lambda_2 + \mu_1 = -1 + 2$;
- -1 (multiplicity 3), obtained in 2 ways: $\lambda_1 + \mu_2 = 1 + (-2)$ and $\lambda_2 + \mu_3 = -1 + 0$;
- 3 (multiplicity 1), obtained as $\lambda_1 + \mu_1$;
- -3 (multiplicity 1), obtained as $\lambda_2 + \mu_2$.

The lattices $L_{H(3,2),3}$ and $L_{H(3,2),3}$ are both similar to $\mathbb{Z}$, however $L_{H(3,2),1}$ is the orthogonal projection of $\mathbb{Z}^8$ onto the space spanned by

$$\left(L_{K_2,1} \otimes_{\mathbb{Z}} L_{C_4,0}\right) \oplus \left(L_{K_2,-1} \otimes_{\mathbb{Z}} L_{C_4,2}\right).$$

This lattice is similar to A_3^*, and the same is true for the lattice $L_{H(3,2),-1}$. This example demonstrates that a product graph construction can generate a lattice that is not a tensor product or direct sum.

Example 4.4.9. Recall the construction of the Kneser graph $KG_{n,k}$: vertices of this graph correspond to k-element subsets of a set of n elements, and two vertices are connected by an edge if the corresponding sets are disjoint. $KG_{n,k}$ has eigenvalue $(-1)^j\binom{n-k-j}{k-j}$ occurring with multiplicity $\binom{n}{j}-\binom{n}{j-1}$ for all $j=1,\dots,k$, and therefore gives rise to lattices in arbitrarily large dimensions. While Kneser graphs are not distance transitive in general, there are some examples that are.

For instance, Petersen graph (which is the same as the Kneser graph $KG_{5,2}$) has 10 vertices and three eigenvalues: 3 (multiplicity 1), 1 (multiplicity 5) and -2 (multiplicity 4). It is distance transitive, and hence generates strongly eutactic lattices corresponding to its eigenvalues. For eigenvalue -2, we obtain the lattice A_4^*. For eigenvalue 1, we obtain A_5^2, an example of the Coxeter-Barnes lattice A_n^r, defined as the lattice contained in the hyperplane $H=(\boldsymbol{e}_1+\cdots+\boldsymbol{e}_{n+1})^\perp$ with the basis

$$\left\{\boldsymbol{e}_1-\boldsymbol{e}_2,\dots,\boldsymbol{e}_1-\boldsymbol{e}_n,\frac{1}{r}\sum_{i=2}^{n+1}(\boldsymbol{e}_1-\boldsymbol{e}_i)\right\}$$

and defined for all positive rational r. When r is an integer dividing $n+1$, these are exactly the lattices Λ for which $A_n\subset\Lambda\subset A_n^*$, so that A_n^r contains A_n to index r ([103], Section 5.2). In particular, A_5^2 is the unique sublattice of the dual lattice

$$A_5^*:=\{\boldsymbol{x}\in\mathbb{R}^5:\boldsymbol{x}^\top\boldsymbol{y}\in\mathbb{Z}\text{ for all }\boldsymbol{y}\in A_5\},$$

which contains A_5 to index 2. As mentioned above, it can be described as a full rank lattice in the hyperplane

$$\left\{\boldsymbol{x}\in\mathbb{R}^6:\sum_{i=1}^{6}x_i=0\right\},$$

identified with $\mathbb{R}^5$. Here is this description:

$$A_5^2=\operatorname{span}_{\mathbb{Z}}\left\{\boldsymbol{e}_1-\boldsymbol{e}_2,\dots,\boldsymbol{e}_1-\boldsymbol{e}_5,\frac{1}{2}\left(5\boldsymbol{e}_1-\sum_{i=2}^{6}\boldsymbol{e}_i\right)\right\},$$

where $\boldsymbol{e}_1, \dots, \boldsymbol{e}_6$ are standard basis vectors in $\mathbb{R}^6$.

Example 4.4.10. The line graph of a graph Γ is the graph Γ' whose vertices correspond to edges of Γ, and two vertices are connected by an edge if and only if the corresponding edges in Γ meet in a vertex. For instance, the line graph of the Petersen graph is a distance transitive graph on 15 vertices. Among its eigenvalues, -1 comes with multiplicity 4 and the corresponding lattice is A_4^*, -2 comes with multiplicity 5 and the corresponding lattice is the Coxeter lattice A_5^3, which can be described as a full rank lattice in the hyperplane

$$\left\{ \boldsymbol{x} \in \mathbb{R}^6 : \sum_{i=1}^{6} x_i = 0 \right\},$$

identified with $\mathbb{R}^5$. Here is the description:

$$A_5^3 = \operatorname{span}_{\mathbb{Z}} \left\{ \boldsymbol{e}_1 - \boldsymbol{e}_2, \dots, \boldsymbol{e}_1 - \boldsymbol{e}_5, \frac{1}{3} \left(5\boldsymbol{e}_1 - \sum_{i=2}^{6} \boldsymbol{e}_i \right) \right\},$$

where $\boldsymbol{e}_1, \dots, \boldsymbol{e}_6$ are standard basis vectors in $\mathbb{R}^6$. It is the unique sublattice of A_5^* containing A_5 to index 3; it is isometric to the dual of A_5^2.

Example 4.4.11. Recall the construction of the Johnson graph $J(n, k)$: vertices of this graph correspond to k-element subsets of a set of n elements, and two vertices are connected by an edge if the corresponding sets intersect in $k - 1$ elements. $J(n, k)$ is a distance transitive graph, which has $\binom{n}{k}$ vertices and eigenvalue $((k - j)(n - k - j) - j)$ occurring with multiplicity $\binom{n}{j} - \binom{n}{j-1}$ for all $j = 1, \dots, \min\{k, n - k\}$, and therefore gives rise to strongly eutactic lattices in arbitrarily large dimensions.

It is well known that Johnson graph $J(n, 2)$ (also known as the triangular graph T_n) is the line graph of the complete graph K_n and the complement of the Kneser graph $KG_{n,2}$. In particular, $J(5, 2)$ is the line graph of K_5 and the complement of the Petersen graph. Further, $J(n, 2)$ is a strongly regular graph, and so always has three eigenvalues: $2(n - 2)$ (multiplicity 1), $n - 4$ (multiplicity $n - 1$), -2 (multiplicity $n(n - 3)/2$). We present some examples of lattices from

$J(n, 2)$ in Table 4.2, which are the same as for its complement $KG_{n,2}$. In this table, the lattice $L_{J(n,2),-2}$ for $n = 6$ is listed as the 9-dimensional lattice `sth15` in the online catalog [102] of strongly eutactic lattices; for larger n in our table these lattices are not catalogued.

$J(n, 2)$	# of vertices	$L_{J(n,2),n-4}$	$L_{J(n,2),-2}$
$J(4, 2)$	(6)	$\mathbb{Z}^3$	A_2
$J(5, 2)$	(10)	A_4^*	A_5^2
$J(6, 2)$	(15)	A_5^3	SE in $\mathbb{R}^9$
$J(7, 2)$	(21)	A_6^*	SE in $\mathbb{R}^{14}$
$J(8, 2)$	(28)	E_7^*	SE in $\mathbb{R}^{20}$
$J(9, 2)$	(36)	A_8^*	SE in $\mathbb{R}^{27}$
$J(10, 2)$	(45)	A_9^5	SE in $\mathbb{R}^{35}$

Table 4.2: Examples of strongly eutactic lattices from Johnson $J(n, 2)$ graphs. "SE" stands for strongly eutactic lattice.

As we we mentioned above, the Johnson graphs $J(n, 2)$ are strongly regular, as are their complements Kneser graphs $KG_{n,2}$. Recall that a (connected) graph Γ on n vertices is called *strongly regular* with parameters k, ℓ, m whenever it is not complete and:

1. each vertex is adjacent to k vertices,
2. for each pair of adjacent vertices there are ℓ vertices adjacent to both,
3. for each pair of non-adjacent vertices there are m vertices adjacent to both.

Strongly regular graphs are known to have many remarkable properties. In particular, these are precisely the k-regular graphs with three distinct eigenvalues. One of these eigenvalues is always k (multiplicity 1) with the vector $(1, \dots, 1)^\top$ being a corresponding eigenvector; the other two eigenvalues are roots of the polynomial $x^2 - (\ell - m)x + (m - k)$, which are known to be integers when they have different multiplicity. See Chapter 9 of [22] for many more details.

Example 4.4.12. We mention a few more examples of notable vertex transitive strongly regular graphs giving rise to interesting lattices (these graphs are described, for instance, in [22] and in [5]).

These examples are all connected by the common property of being graphs represented by the roots of the lattice E_8 (along with some others already described above; see Section 3.11 of [23], also Section 14.3 of [46]).

The folded 5-cube obtained by identifying the antipodal vertices of the 5-cube is a distance transitive and strongly regular graph on 16 vertices with parameters $k = 5,\ \ell = 0,\ m = 2$. Its complement (also distance transitive and strongly regular) is called the Clebsch graph. They each have an eigenvalue of multiplicity 5 (-3 and 2, respectively), and the corresponding lattice is D_5^*, the dual of the root lattice D_5, where the lattice family D_n is defined as

$$D_n = \left\{ \boldsymbol{x} \in \mathbb{Z}^n : \sum_{i=1}^{n} x_i \equiv 0 \pmod 2 \right\}.$$

The Shrikhande graph can be constructed as Cayley graph of the group $\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$, taking elements for vertices and connecting two vertices by an edge if and only if their difference is in $\{\pm(1,0), \pm(0,1), \pm(1,1)\}$. This graph is a vertex transitive, but not distance transitive, and strongly regular graph on 16 vertices with parameters $k = 6,\ \ell = 2,\ m = 2$. It has an eigenvalue 2 of multiplicity 6, and the corresponding lattice is D_6^+, which is an example of one of the lattices

$$D_n^+ = D_n \cup \left(\frac{1}{2} \sum_{i=1}^{n} \boldsymbol{e}_i + D_n \right),$$

defined for even n. The complement of the Shrikhande graph (also vertex transitive, but not distance transitive, and strongly regular) has eigenvalue -3 with multiplicity 6 and produces the same lattice. Notice that even though the graphs are not distance transitive, the generated lattice is still strongly eutactic.

The Schläfli graph is the complement of the intersection graph of the 27 lines on a cubic surface. It is a distance transitive and strongly regular graph on 27 vertices with parameters $k = 16,\ \ell = 10,\ m = 8$ and has eigenvalue 4 of multiplicity 6. Its complement (also distance transitive and strongly regular) has eigenvalue -5 with multiplicity 6. Both of these generate the lattice E_6^*, the dual of the root lattice E_6. Recall that the lattice $E_8 = D_8^+$, the lattice E_7 is the sublattice of E_8 with $x_7 = x_8$, and the lattice E_6 is the sublattice of E_8 with $x_6 = x_7 = x_8$ (see [36] for more details).

Finally, the Gosset graph (the only one out of these E_8-root graphs which is not strongly regular) is a distance transitive graph on 56 vertices that can be identified with two copies of the set of edges of the complete graph K_8. Then two vertices from the same copy of K_8 are connected by an edge if they correspond to disjoint edges of K_8, and two vertices from different copies of K_8 are connected by an edge if they correspond to edges that meet in a vertex (see [23] for more details). The Gosset graph has eigenvalue 9 of multiplicity 7, generating the lattice E_7^*, the dual of E_7.

The main purpose of all these examples is to demonstrate that this construction of strongly eutactic lattices from distance transitive (and possibly from vertex transitive) graphs appears to produce a wide range of interesting examples already in low dimensions, and hence may be quite useful in higher dimensions too where a classification of strongly eutactic lattices is not yet available.

We also observe here an interesting connection between contact polytopes of some lattices and graphs generating them. For a lattice Λ, its contact polytope $C(\Lambda)$ is defined as the convex hull of the set of minimal vectors. The significance of the contact polytope is that its vertices are points on the sphere centered at the origin in the sphere packing associated to Λ at which neighboring spheres touch it. Hence the number of vertices of $C(\Lambda)$ is the kissing number of Λ. The skeleton graph of this polytope $\mathrm{skel}(C(\Lambda))$ is the graph consisting of vertices and edges of $C(\Lambda)$.

Let us consider an example $\Lambda = E_6^*$. The contact polytope of E_6^* has 54 vertices, split into 27 $\pm$ pairs: it is a diplo-Schläfli polytope (see [37]). The prefix "diplo" means double: for a polytope Π a diplo-Π polytope is a polytope whose vertices are vertices of Π and its opposite $-\Pi$. The Schläfli polytope, with Coxeter symbol 2_{21}, has 27 vertices corresponding to the 27 lines on a cubic surface [39]. Its skeleton is the Schläfli graph Γ. By Example 4.4.12 above, Γ has an eigenvalue 4 of multiplicity 6, and $L_{\Gamma,4} = E_6^*$.

Here is another example of this dual correspondence. For $\Lambda = E_7^*$, its contact polytope is the Gosset polytope (also called Hess polytope) 3_{21}, which has 56 vertices (see [68], [38]). Its skeleton is the Gosset graph Γ. As we know from Example 4.4.12 above, Γ has an eigenvalue 9 of multiplicity 7, and $L_{\Gamma,9} = E_7^*$.

This kind of correspondence certainly does not work for all strongly eutactic lattices. For instance, the contact polytope of A_n^* is a diplo-simplex (see [37]), and the skeleton graph of a regular simplex on $n+1$ vertices is the complete graph K_{n+1}. By Lemma 4.4.3, K_{n+1} generates A_n, but not A_n^*. On the other hand, the diplo-simplex for A_3^* is a cube, whose skeleton graph Q_3 is isomorphic to $H(3,2)$ and the lattice corresponding to eigenvalue 1 (or -1) is A_3^* (see Example 4.4.8 above). It would be interesting to understand this correspondence better.

4.5 On the coherence of a lattice

We conclude with some remarks on the coherence of lattices and frames and their use in the application of compressed sensing. While this discussion is speculative, we hope it will also draw interesting connections and spark interesting future directions. We start with some definitions. Let $L \subset \mathbb{R}^n$ be a lattice. As usual, let $S(L)$ be the set of minimal vectors of L, which come in $\pm$ pairs, and let us write $S^*(L)$ for the subset of $S(L)$ where only one vector of each pair is included. Then any two vectors $\boldsymbol{x}, \boldsymbol{y} \in S^*(L)$ are linearly independent, so the angle $\vartheta(\boldsymbol{x}, \boldsymbol{y})$ between them is in the interval $[\pi/3, 2\pi/3]$. Define the *coherence* of L to be

$$C(L) := \max\{|\cos\vartheta(\boldsymbol{x}, \boldsymbol{y})| \colon \boldsymbol{x} \neq \boldsymbol{y} \in S^*(L)\},$$

then $0 \leq C(L) \leq \frac{1}{2}$.

Coherence plays an important role in many applications, and ETFs with small coherence have attracted attention for being potentially useful. For example, the field of *compressed sensing* aims to recover a sparse vector from a small number of linear measurements. The applications are abundant, ranging from medical imaging and environmental sensing to radar and communications [57, 85]. Here, we say a vector is s-sparse when it has at most s non-zero entries. Put succinctly, compressed sensing aims to recover an s-sparse vector $x \in \mathbb{R}^n$ from the measurements $y = Ax \in \mathbb{R}^k$, where

A is a suitable $k \times n$ measurement matrix. It is now well known that an s-sparse vector x can be efficiently and robustly recovered from measurements y when the number of measurements k is approximately $s \log n$, yielding a significant reduction in the dimension of the representation from n to $s \log n$ (since s is typically much smaller than n).

For such techniques, one typically constructs A randomly and/or asks that the matrix has highly incoherent columns; this is equivalent to requiring $C(L)$ to be small in situations when columns of A are minimal vectors of a lattice L. To this end, it is very natural to consider ETFs and other frames with nice algebraic properties as suitable measurement operators [146, 61]. Moreover, in many applications, more is known about the signal than simple sparsity; for example, the signal may often also have integer-valued entries or entries in some other lattice. Such is the case for example in wireless communications [125], collaborative filtering [42], error correcting codes [27], and many others. Although there is some preliminary work for this setting [99, 47, 138, 144, 163, 55], there is still not a rigorous understanding of when and how the lattice structure of the signal can actually be utilized in reconstruction.

Our work may shed some light on integer-valued sparse recovery by observing the following. If the integer span of an ETF or another suitable frame is a lattice, then viewing this frame as a measurement matrix (whose columns are the frame vectors), its image restricted to integer-valued signals forms a lattice. This allows for separation of such images of sparse signals, analogous to the well-known Johnson-Lindenstrauss lemma, which has been used to guarantee accurate recovery in compressed sensing [11]. In fact, when the minimal vectors of the lattice contain the frame vectors, this separation can be bounded. Viewed in this context, Theorem 4.1.1 gives an answer as to which measurement matrices (given as tight frames) map integer-valued signals to elements of a lattice. Studies of properties of such lattices (e.g. Voronoi cell) have the potential to give stronger guarantees in the integer sparse regime for reconstruction. Of course the integer span of vectors is a larger subset than the image of sparse vectors, however it may be interesting future work to specialize these questions to integer vectors that are in particular also sparse. Group frames may also be interesting for further study given the advantage they give due to their compact representation:

fixing a group and picking a starting vector, the entire frame can be generated as its orbit under the group action.

To examine how deterministic low-coherence measurement matrices perform in the integer sparse framework we perform a simple experiment using a Steiner ETF of 4000 vectors in $\mathbb{R}^{775}$, generated from the incidence matrix of an affine Steiner triple system. A schematic representation of this ETF and its Gram matrix is shown in Figure 4.2. We chose this measurement matrix for these experiments for a couple of reasons. Steiner ETFs, ETFs generated from a type of combinatorial construction, have been singled out as some of the ETFs with the most potential in application to problems in compressed sensing [52].

These Steiner ETFs stand out because by working in a sufficiently large dimension the coherence can be made arbitrarily small and the redundancy as large as desired, this property being inherited from known constructions of Hadamard matrices and Steiner triple systems used to generate these incoherent frames [52, 67]. Although these matrices have other undesirable properties such as being sparse themselves, the freedom to generate large matrices with small coherence is instrumental in sparse recovery given the well-studied relation between low-coherence matrices and guarantees in compressed sensing.

Denoting this frame of vectors by F, we acquire the measurements $y = Fx$ or the noisy measurements $y = Fx + e$ where x is a vector of varying sparsity and e is scaled Gaussian noise. We then use various compressed sensing algorithms to recover $\hat{x}$ and calculate how often recovery is exact ($x = \hat{x}$) in the noiseless case, and the magnitude of the recovery error ($\|x - \hat{x}\|_2$) in the noisy case. We show results for the simple least-squares method (LS) that simply sets $\hat{x} = F^{\dagger}y$, basic hard thresholding (HT) which first estimates the support of x via the proxy $F^T y$ and then performs least-squares over that support, Orthogonal Matching Pursuit [145] (OMP) which is an iterative greedy algorithm, and PrOMP [55] which is a modification of OMP for integer-valued signals. The results are shown in Figure 4.3, where we see unsurprisingly that PrOMP performs quite well in this case, confirming the previous observations of effectiveness of pre-processing steps in lattice-valued compressed sensing.

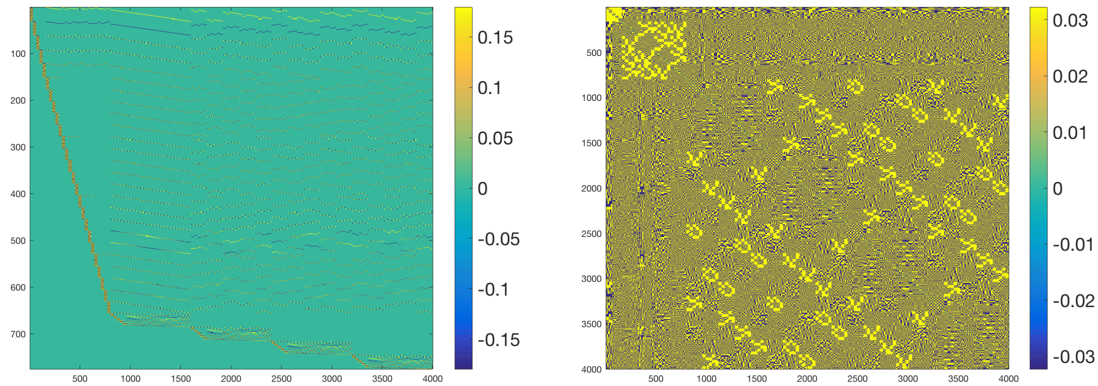

Figure 4.2: Left: A plot of entries in the Steiner ETF. Right: The corresponding ‘hollow’ Gram matrix $(A^\top A - I)$.

The previous analysis in [55] has explained via a concentration of measure argument why this should hold for Gaussian matrices, but numerically there is some evidence that performance improvements hold for deterministic measurements and integer signals in iterative compressed sensing procedures when a pre-processing step, as is found in PrOMP, is applied. [a]

[a]Chapter adapted from the paper [60].

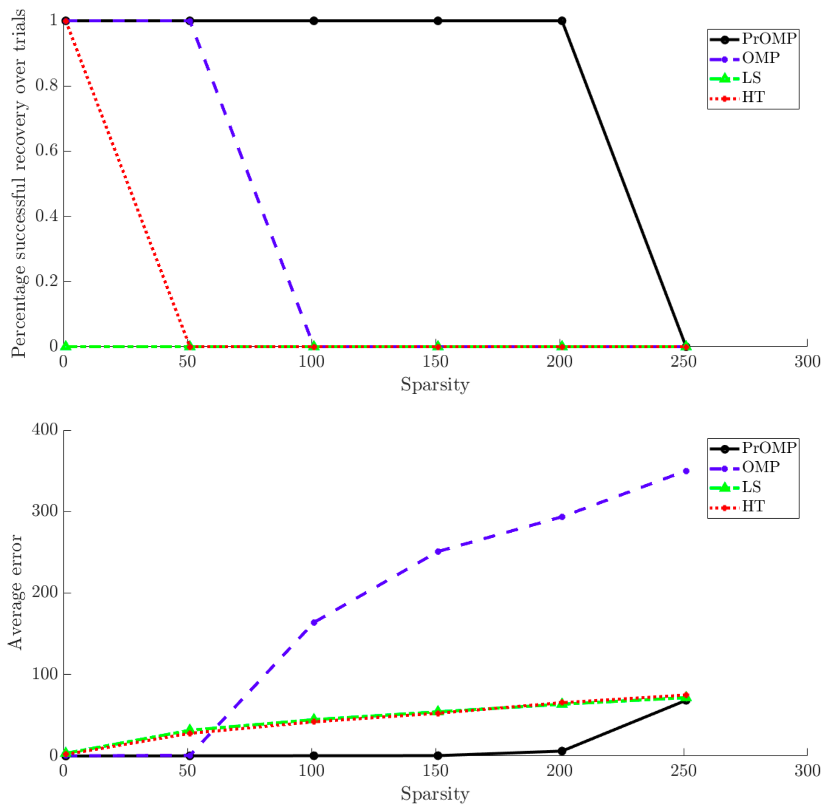

Figure 4.3: Recovery results for various algorithms (PrOMP, OMP, Hard Thresholding, Least Squares) using a Steiner ETF in $\mathbb{R}^{775}$, size 4000, as the measurement matrix. Top: Percentage of accurate recovery. Bottom: Noise added to the measurements to have norm 0.1.

Appendices

APPENDIX A

TABLES AND PROGRAMS FOR CHAPTER 2

A.1 Configuration table, numerical LP bounds, and solutions to variational principle

A.1.1 Parameters of the conjectured and rigorous optimizing configurations

Table A.1 gives weights and inner products of the support vectors of p-frame minimizing measures in $\mathbb{R}^d$, see Table 2.1 and Section 2.5.2.

Table A.1: Optimal and conjectured configurations for p-frame energies. The configurations are supported on N unit norm vectors in $\mathbb{R}^d$, and are strength M designs. Only the absolute values of inner products are given. Note: $\alpha = \frac{\sqrt{75+30+\sqrt{5}}}{15}$, $\beta = \sqrt{\frac{1}{15}(5-2\sqrt{5})}$, and $\gamma = \frac{\sqrt{6-2\sqrt{5}}}{6}$.

d	N	M	Weights	Inner Products	Name
2	N	$N-1$	$1/N$	$\lvert\cos(2\pi j/N)\rvert, 1 \leq j < N$	$2N$-gon
d	d	1	$1/N$	0	cross polytope
3	6	2	$1/N$	$\frac{1}{\sqrt{5}}$	icosahedron
3	11	3	$\frac{1}{10}, \frac{2}{27}, \frac{49}{540}$	$0, \frac{1}{7}, \frac{4}{7}, \frac{5}{7}, \sqrt{\frac{1}{7}}, \sqrt{\frac{3}{7}}, \sqrt{\frac{4}{7}}$	Reznick weighted design
3	16	4	$\frac{5}{84}, \frac{9}{140}$	$\frac{1}{3}, \frac{1}{\sqrt{5}}, \sqrt{\frac{5}{9}}, \alpha, \beta$	icosahedron and dodecahedron
4	11	2	$\frac{1}{10}, \frac{3}{32}, \frac{3}{40}$	$\frac{1}{3}, \frac{\sqrt{2}}{3}, \frac{\sqrt{6}}{6}, \frac{\sqrt{5}+1}{6}, \gamma$	weighted design
4	24	3	$1/N$	$0, 1/2, 1/\sqrt{2}$	D_4 roots
4	60	5	$1/N$	$0, \frac{\sqrt{5}\pm 1}{4}, \frac{1}{2}$	600-cell
5	16	2	$\frac{5}{84}, \frac{9}{140}$	$\frac{1}{5}, \frac{1}{3}, \frac{1}{\sqrt{5}}$	hemicube
5	41	3	$\frac{25}{1008}, \frac{8}{315}, \frac{2}{105}$	$0, \frac{1}{5}, \frac{1}{2}, \frac{3}{5}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{5}}, \sqrt{\frac{2}{5}}$	Stroud weighted design
6	22	2	$\frac{3}{64}, \frac{1}{24}$	$0, \frac{1}{3}, \frac{1}{\sqrt{6}}$	cross polytope and hemicube
6	63	3	$\frac{2}{135}, \frac{1}{60}$	$0, \frac{1}{4}, \frac{1}{2}, \sqrt{\frac{3}{8}}$	E_6 and E_6^* roots
7	28	2	$1/N$	$1/3$	kissing E_8
7	91	3	$\frac{3}{308}, \frac{8}{693}$	$0, \frac{1}{27}, \frac{1}{8}, \frac{\sqrt{3}}{9}$	E_7 and E_7^* roots
8	36	1	$1/N$	$5/14, 2/7$	mid-edges of regular simplex
8	120	3	$1/N$	$0, 1/2$	E_8 roots
23	276	2	$1/N$	$1/5$	equiangular
23	2300	3	$1/N$	$0, 1/3$	kissing Λ_{24}
24	98280	5	$1/N$	$0, 1/4, 1/2$	Λ_{24} minimal vectors

A.1.2 Numerical LP bounds

Table A.2 collects linear programming lower bounds corresponding to small values of d and odd values p for the p-frame energy on $\mathbb{S}^{d-1}$. These may be compared to the numerical/proved upper bounds presented earlier, as is done partially in Table 2.4.

Table A.2: Numeric linear programming lower bounds for odd-valued p-frame energies.

d	$p=3$	$p=5$	$p=7$
3	0.2412	0.1655	0.1248
4	0.1612	0.09607	0.06454
5	0.1170	0.06169	0.03740
6	0.08970	0.04240	0.02344
7	0.07142	0.03060	0.01556
8	0.05852	0.02291	0.01080
9	0.04902	0.01770	0.007768
10	0.04180	0.01401	0.005750
11	0.03616	0.01131	0.004360
12	0.03166	0.009290	0.003375
13	0.02801	0.007737	0.002658
14	0.02499	0.006524	0.002125
15	0.02248	0.005561	0.001721
16	0.02035	0.004785	0.001413
17	0.01853	0.004152	0.001171
18	0.01696	0.003630	0.0009813
19	0.01559	0.003195	0.0008280
20	0.01440	0.002830	0.0007054
21	0.01335	0.002520	0.0006047
22	0.01242	0.002256	0.0005217
23	0.01159	0.002028	0.0004529
24	0.01085	0.001832	0.0003952

In the below lines, we give the certificate (polynomials) for each of the linear programming lower bounds for p-frame energies in the table above. The first (constant) term in each list gives the bound, while the remaining values are the full coefficients of the polynomial in the Jacobi polynomial basis.

Coefficients for $p = 3$

```
3-[0.2412022, 1.2336106, 0.4046283,         0, 0.0355815,         0,         0]
```

```
4-[0.1612372, 1.2980505,  0.607158,         0, 0.0000032, 0.0000006, 0.0000005]
5-[0.1170619, 1.2887887, 0.7951451,         0, 0.0000006, 0.0000001, 0.0000002]
6-[0.0897087, 1.2585643, 0.9634589, 0.0000001, 0.0000006, 0.0000002, 0.0000009]
7-[0.07142850, 1.2207883, 1.1136198,         0, 0.0000004, 0.0000002, 0.0000005]
8-[0.0585221, 1.1810586, 1.2478157, 0.0000001, 0.0000008, 0.0000008, 0.0000016]
9-[0.0490232, 1.1418502, 1.3681835, 0.0000002, 0.0000013, 0.0000012,  0.000004]
10-[0.0418006, 1.1042717, 1.4765936,         0, 0.0000002, 0.0000005, 0.0000009]
11-[0.0361628, 1.0687456, 1.5747011,         0, 0.0000009, 0.0000009, 0.0000016]
12-[0.0316658, 1.0353921, 1.6638929, 0.0000001,  0.000001, 0.0000011, 0.0000018]
13-[0.0280131, 1.0041817, 1.7453274,         0, 0.0000001, 0.0000002, 0.0000006]
14-[0.0249999, 0.9750019, 1.8199955,         0, 0.0000002, 0.0000005, 0.0000009]
15-[0.0224812, 0.9477157, 1.8887272,         0, 0.0000004, 0.0000007, 0.0000011]
16-[0.0203512, 0.9221891, 1.9522021, 0.0000001,  0.000001, 0.0000015, 0.0000025]
17-[0.0185315, 0.898274, 2.0110284, 0.0000001, 0.0000007,  0.000001, 0.0000018]
18-[0.0169629, 0.8758297,  2.065723, 0.0000004, 0.0000014,  0.000002, 0.0000033]
19-[0.0155997, 0.8547412,   2.11671, 0.0000002, 0.0000011, 0.0000019, 0.0000039]
20-[0.0144066, 0.8348942, 2.1643648, 0.0000001, 0.0000004, 0.0000012, 0.0000033]
21-[0.0133556, 0.8161776, 2.2090266, 0.0000004, 0.0000009, 0.0000032, 0.0000106]
22-[0.0124241, 0.7984992, 2.2509808, 0.0000007, 0.0000017, 0.0000064, 0.0000182]
23-[0.0115942, 0.7817578, 2.2905177, 0.0000001, 0.0000005, 0.0000012, 0.0000054]
24-[0.0108511, 0.7659088, 2.3277844, 0.0000002, 0.0000006, 0.0000016, 0.0000064]
```

Coefficients for $p = 5$

```
3-[ 0.165583, 1.034617, 0.837685, 0.139628,            0, 0.017831, 0.000001]
4-[ 0.0960763, 0.9593817, 1.1580828, 0.2545875,         0, 0.0515163, 0.0000008]
5-[ 0.0616939, 0.8611382, 1.3973619, 0.3801922, 0.0000001, 0.1165704, 0.0000008]
6-[ 0.0424024, 0.7671555, 1.5707189, 0.50520640, 0.0000002, 0.2273608,  0.000001]
7-[ 0.0306037, 0.6835527, 1.6919203, 0.6204386, 0.0000015, 0.4010393, 0.0000071]
8-[ 0.0229166, 0.6212031, 1.8318931, 0.8027256, 0.0000008, 0.1745087, 0.0000031]
9-[ 0.0177062, 0.5641381, 1.9308417, 0.9832606,  0.000001, 0.0000304, 0.0000042]
10-[  0.014014, 0.5117733, 1.9870142, 1.1302673, 0.0000009, 0.0000166, 0.0000047]
11-[ 0.0113149, 0.4665424, 2.0270676, 1.2733324, 0.0000013, 0.000011, 0.0000054]
12-[   0.00929, 0.4272722,  2.054648, 1.4118708, 0.0000019, 0.0000108, 0.0000072]
```

```
13-[ 0.0077373, 0.3929873, 2.0725144, 1.5455775, 0.0000023, 0.0000165, 0.0000102]
14-[ 0.0065243, 0.3628894, 2.0827903, 1.6743161, 0.0000025, 0.0000182, 0.0000121]
15-[  0.005561, 0.3363239, 2.0870975, 1.7980908,  0.000003, 0.0000207, 0.0000152]
16-[ 0.0047851, 0.3127549, 2.0866892, 1.9169021, 0.0000194, 0.0001486, 0.0001159]
17-[ 0.0041524, 0.2917414,  2.082556, 2.0310784, 0.0000289, 0.0001517, 0.0001296]
18-[ 0.0036305, 0.2729298, 2.0755535,  2.14055,  0.000032, 0.0001561, 0.0001479]
19-[ 0.0031957, 0.2560063, 2.0661881, 2.2457202, 0.0000379, 0.0001683, 0.0001675]
20-[ 0.0028303, 0.2407256, 2.0550066, 2.3467218, 0.0000331, 0.0001592,  0.000164]
21-[ 0.0025206, 0.2268771, 2.0424088, 2.443697, 0.0000326, 0.0001442, 0.0001622]
22-[ 0.0022562, 0.2142807, 2.0286867, 2.5369098, 0.0000339, 0.0001129, 0.0001392]
23-[ 0.0020289, 0.2027851, 2.0140921, 2.6265819, 0.0000259, 0.0000767, 0.0000941]
24-[ 0.001832, 0.192269, 1.998926, 2.712601, 0.000034, 0.000097, 0.000128]
```

Coefficients for $p = 7$

```
3-[ 0.12484054, 0.87385072, 0.98284208,  0.4056134, 0.04283021, 0, 0.00379165, 8.72E-4, 4E-8]
4-[ 0.06454795, 0.73921879, 1.26270856,  0.7059021, 0.09381929, 4E-8, 0.01177475, 2.3444E-3, 3.4E-7]
5-[ 0.03740246, 0.61070194, 1.42641859, 1.01769222, 0.16385056, 3.7E-7, 0.02628529, 2.76862E-3, 1.46E-6]
6-[   0.02344, 0.5046257, 1.5113796, 1.3209008, 0.2504716, 6E-7, 0.0497021, 1.62E-4, 2.4E-6]
7-[ 0.01556243, 0.41985945, 1.54398287, 1.60327732, 0.34876063, 1.08E-6, 0.09157963, 6.94E-6, 4.22E-6]
8-[ 0.01080222, 0.35247062, 1.54294606, 1.86036077,  0.4552268, 1.84E-6,  0.1556982, 9.13E-6, 8.39E-6]
9-[ 0.00776849, 0.29861957, 1.52035926, 2.09031709, 0.56593773, 2.46E-6, 0.24897724, 1.391E-5, 1.972E-5]
10-[ 0.00575078, 0.25521552, 1.48419517, 2.29309301, 0.67712853, 3.29E-6, 0.37919287, 2.441E-5, 2.264E-6]
11-[ 0.00436094, 0.21989327, 1.43971032, 2.46942635,   0.784679, 8.28E-6, 0.55653755, 7.41E-5, 1.1333E-4]
12-[ 0.00337508, 0.19086672, 1.39038704, 2.62058395, 0.88513044,  1.72E-5, 0.79073546, 1.4585E-4, 2.4427E-4]
13-[ 0.0026581,  0.166789, 1.3385353, 2.7479668, 0.9751261,  1.9E-5, 1.0924305, 1.481E-4, 2.815E-4]
14-[ 0.00212531,  0.1466367, 1.28563212, 2.85266154, 1.05049581, 1.987E-5, 1.47644544, 1.4473E-4, 3.3834E-4]
15-[ 0.00212531,  0.1466367, 1.28563212, 2.85266154, 1.05049581, 1.987E-5, 1.47644544, 1.4473E-4, 3.3834E-4]
16-[  0.001413, 0.1166988,  1.211958, 3.2070818, 1.6397564,  7.4E-5, 0.0067668, 5.168E-4, 8.735E-4]
17-[ 0.00117199, 0.10445448, 1.16581167, 3.29923017, 1.79452033, 1.281E-5, 0.00081233, 1.3952E-4, 3.6515E-4]
18-[ 0.0009813,  0.093918,  1.121319, 3.3794104, 1.9459159, 5.65E-5, 0.0030266, 6.613E-4, 1.7487E-3]
19-[ 0.000828, 0.084799, 1.07869, 3.449584, 2.096244, 1.58E-4, 0.004206, 1.291E-3, 3.022E-3]
20-[ 0.0007054, 0.0768699, 1.0380701, 3.5113247, 2.2453321, 1.179E-4, 0.0035763, 1.4601E-3, 3.913E-3]
21-[ 0.0006047, 0.0699328, 0.9993427, 3.5649714, 2.3925271, 1.554E-4,  0.003356, 1.7324E-3, 4.2666E-3]
```

```
22-[ 0.0005217,  0.063836, 0.9625032, 3.6115992,  2.538303, 1.642E-4, 0.0022875, 1.4165E-3, 3.4323E-3]
23-[ 0.0004529, 0.0584566, 0.9275334, 3.6520877, 2.6804131, 1.215E-4, 0.0027075, 1.4009E-3, 5.1695E-3]
24-[ 0.0003952, 0.0536864, 0.8942927, 3.6867572,  2.820459, 1.518E-4, 0.0030378, 1.7802E-3, 6.192E-3]
```

A.1.3 Causal variational principle

Cross-polytope

Let the following polynomial be given,

$$H(t) = 8t^2 + 8t.$$

It is easy to see that H is positive definite on $\mathbb{S}^2$. Additionally, it is obvious that

$$H(t) \leq \mathcal{L}(t) \qquad \text{for all } t \in [-1, 1],$$

and

$$H(-1) = \mathcal{L}(-1) = 0, \quad H(0) = \mathcal{L}(0) = 0, \quad H(1) = \mathcal{L}(1) = 16,$$

so that H coincides with $\mathcal{L}$ on the set $\{x \cdot y : x, y \in \operatorname{supp} \nu\}$.

We obtain that for any measure $\mu \in \mathcal{P}$,

$$I_{\mathcal{L}}(\mu) \geq I_H(\mu) \geq I_H(\sigma) = I_H(\nu) = I_{\mathcal{L}}(\nu), \tag{A.1.1}$$

where we have used the fact that $H(t) \leq \mathcal{L}(t)$ for $t \in [-1, 1]$, so $I_{\mathcal{L}}(\mu) \geq I_H(\mu)$. Since H is positive definite, according to Propositions 2.2.2 and 2.2.3, we have that σ minimizes I_H, i.e. $I_H(\mu) \geq I_H(\sigma)$. We have also used that the cross-polytope is a 3-design and H is a quadratic polynomial, hence $I_H(\sigma) = I_H(\nu)$. Finally, $H(t) = \mathcal{L}(t)$ for $t \in \{x \cdot y : x, y \in \operatorname{supp} \nu\} = \{0, \pm 1\}$, hence $I_H(\nu) = I_{\mathcal{L}}(\nu)$. This proves that the cross-polytope minimizes $I_{\mathcal{L}}$ for $\tau = \sqrt{2}$.

Icosahedron

We shall need two facts about the icosahedron, namely that the set of inner products between elements of $\mathcal{C}$ is $\{x \cdot y : x, y \in \mathcal{C}\} = \left\{\pm 1, \pm 1/\sqrt{5}\right\}$, and that the icosahedron $\mathcal{C}$ is a 5-design. For simplicity let us consider the function $F(t) = \frac{\mathcal{L}(t)}{\mathcal{L}(1)}$ so that $F(1) = 1$ (obviously, this does not effect the minimizers).

We construct the following polynomial:

$$\begin{aligned} H(t) &= \frac{5(5-\sqrt{5})}{32} t^4 + \frac{5}{8} t^3 + \frac{3\sqrt{5}-5}{16} t^2 - \frac{1}{8} t + \frac{1-\sqrt{5}}{32} \\ &= \frac{5-\sqrt{5}}{28} C_4(t) + \frac{1}{4} C_3(t) + \frac{20+3\sqrt{5}}{84} C_2(t) + \frac{1}{4} C_1(t) + \frac{1}{12} C_0(t), \end{aligned}$$

where C_k are the standard Legendre polynomials. We observe then that H is positive definite, and that $H(t) \leq F(t)$ for $-1 \leq t \leq 1$, which follows from the formula

$$H(t) = \frac{5}{32}(5-\sqrt{5})(t+1)(t-\frac{1}{\sqrt{5}})(t+\frac{1}{\sqrt{5}}).$$

A glance at this formula gives $H \leq F$ for $t \in [-1, \frac{1}{\sqrt{5}}]$, and the fact that $F - H$ is a polynomial with roots

$$t = -1, \frac{1}{\sqrt{5}}, \frac{-1 \pm 4\sqrt{10+4\sqrt{5}}}{\sqrt{5}},$$

gives $H \leq F$ for $t \in [\frac{1}{\sqrt{5}}, 1]$ which is a subset of the interval $[\frac{1}{\sqrt{5}}, \frac{-1+4\sqrt{10+4\sqrt{5}}}{\sqrt{5}}]$.

H coincides with F (by construction) on the set $\{\langle x, y\rangle : x, y \in \mathcal{C}\} = \left\{\pm 1, \pm 1\sqrt{5}\right\}$. H has a local maximum at $-\frac{1}{\sqrt{5}}$ and has been obtained by solving the linear equations $H(t) = F(t)$ for $t = \pm 1, \pm 1/\sqrt{5}$, as well as $H'(-1/\sqrt{5}) = 0$. The same argument as in the previous subsection finally shows

$$I_F(\nu) = \inf_{\mu \in \mathcal{P}} I_F(\mu),$$

i.e. the icosahedron minimizes the energy $I_{\mathcal{L}}$ for $\tau^2 = \frac{2\sqrt{5}}{\sqrt{5}-1}$.

A.2 600-cell is optimal for p-frame energies with $p \in [8, 10]$

As discussed in Section 4, in order to prove optimality of the 600-cell, it suffices to find an Hermite interpolating polynomial for the kernel function, agreeing with it at the scalar products of the 600-cell, and show that it is positive definite. It is done here by showing that the Jacobi coefficients of the polynomial h are positive.

A.2.1 Spanning a polynomial by the Jacobi basis

Instead of minimizing the p-frame energy on $\mathbb{S}^3$, we symmetrize measures under consideration and minimize

$$\iint_{\mathbb{RP}^3} \left(\frac{\tau(x,y)+1}{2}\right)^{p/2} d\mu(x)d\mu(y)$$

Recall that here $\tau(x,y) = \cos(\vartheta(x,y))$, and ϑ denotes the geodesic distance renormalized to $[0, \pi]$.

[1]:
```
a = 1/2

b = -1/2


scalar_prods = [1,(sqrt(5)-1)/4, -1/2, -(sqrt(5)+1)/4, -1]
```

[2]:
```
A = [var('h_%d'%i) for i in (0..8)]

p,t = var('p t')
```

h is a polynomial spanned by Jacobi poynomials $C_n^{(\frac{1}{2},-\frac{1}{2})}(t)$, $n = 0, \ldots, 8; n \neq 6$:

$$h = \left(\sum_{n=0}^{5} + \sum_{n=7}^{8}\right) h_n\, C_n^{\left(\frac{1}{2},-\frac{1}{2}\right)}(t).$$

[3]:
```
h = symbolic_expression(0)

for i in (0..5):

    h += A[i]*jacobi_P(i,a,b,t)
```

```
for i in (7..8):
    h += A[i]*jacobi_P(i,a,b,t)
```

Derivative of h:

```
[4]: hprime = diff(h,t)
```

A.2.2 Interpolation

Let f be the kernel of the symmetrized problem

```
[5]: f = ((t+1)/2)^(p/2)
     fprime = diff(f, t)
```

Jacobi coefficients of the interpolating polynomial are found from the Hermite interpolation conditions. f and h must agree at all the scalar products, and their derivatives must be equal at all the inner products except the endpoints ± 1:

```
[6]: inter0 = [f.subs(t=s)==h.subs(t=s) for s in scalar_prods]
     inter1 = [fprime.subs(t=s)==hprime.subs(t=s) for s in␣
      ↪scalar_prods[1:-1]]
     interpolate = inter0 + inter1
```

```
[7]: coeffs_sol = solve(interpolate, A)[0]
```

Coefficients $h_0, \dots h_8$ as functions of p:

```
[8]: coeffs = [c.rhs() for c in coeffs_sol]
```

A.2.3 Interval arithmetic and derivative bounds

We shall carry out all the non-symbolic computations in the interval arithmetic. First, we set the format for the output of a computation as an interval.

```
[9]: sage.rings.real_mpfi.printing_style = 'brackets'
```

We shall need a bound on the absolute value of the derivative of h_i. It is obtained by expanding the expression for h_i into a sum, then replacing every term in the sum by its maximal absolute value on $[8, 10]$. Finally, all the absolute values are summed up using triangle inequality.

Summands of $\frac{dh_i}{dp}$ are easy to estimate by monotonicity. After the *expand* command, derivative cprime is a sum of several summands, each of which is a product of factors, monotonic on $[8, 10]$. We exploit this structure by replacing every (positive) factor with its maximal value. deriv_bound is obtained by summing up the absolute values of the operands of cprime.

[10]:
```
deriv_bounds = []
for c in coeffs:
    cprime = diff(expand(c),p)

    csub = cprime.subs((1/8*sqrt(5) + 3/8)^(1/2*p)==(1/
 ↪8*sqrt(5) + 3/8)^(1/2*RIF(8))
              ).subs(4^(1/2*p)==4^(1/2*RIF(8))
                    ).subs((-1/8*sqrt(5) + 3/8)^(1/2*p)==(-1/
 ↪8*sqrt(5) + 3/8)^(1/2*RIF(8))
                          ).subs(p=RIF(10))

    deriv_bound = symbolic_expression(0)
    for o in csub.operands():
        deriv_bound += abs(o)
    deriv_bounds.append(deriv_bound.n())
```

[11]:
```
deriv_bounds
```

[11]:
```
[[0.0087005417083128554 .. 0.0087005417083128624],
 [0.047361713211055700 .. 0.047361713211055756],
 [0.55132836870505053 .. 0.55132836870505131],
 [0.35935531675387016 .. 0.35935531675387062],
```

```
[0.11947865468048061 .. 0.11947865468048075],
[0.04979605965982272 .. 0.04979605965982279],
0.000000000000000,
[0.11683357091076153 .. 0.11683357091076168],
[0.57387047207011121 .. 0.57387047207011200]]
```

It follows that derivatives of all the coefficients are uniformly bounded on $[8, 10]$ by e.g. 0.6.

A.2.4 Positivity of coefficients

Bounding coefficients $h_0, \ldots, h_4$ away from zero

Check that the coefficients $h_0, \ldots, h_4$ are positive at $p = 8$:

```
[12]: [coeffs[i].subs(p=RIF(8)).n() for i in (0..4)]
```

```
[12]: [[0.054687500000000000 .. 0.054687500000000028],
 [0.21875000000000002 .. 0.21875000000000025],
 [0.20833333333333292 .. 0.20833333333333426],
 [0.087499999999999633 .. 0.087500000000000522],
 [0.014285714285714123 .. 0.014285714285714430]]
```

The last three h_5, h_7, h_8 are equal to zero at $p = 8$, and so will requre somputing the second derivative.

```
[13]: [coeffs[i].subs(p=RIF(8)).n() for i in [5,7,8]]
```

```
[13]: [[-2.0816681711721686e-17 .. 1.3877787807814457e-17],
 [-1.6653345369377349e-16 .. 1.3877787807814457e-16],
 [-7.7715611723760958e-16 .. 4.4408920985006262e-16]]
```

For the first set of coefficients we proceed as follows. Since the first derivative of h_n is bounded by 0.6, if for some p_0, $h_n(p_0) > 0$, then the same applies to $h_n(p_0 + h_n(p_0))$, and also

$$h_n(p) > 0, \qquad p \in [p_0, p_0 + h_n(p_0)].$$

The loop below iterates this argument, and stops once p has reached the value 10.

[14]:
```
for n in range(5):
    c = coeffs[n]
    p_it = RIF(8)
    numit = 0
    while p_it <= RIF(10):
        p_it = p_it + c.subs(p = p_it).n()
        numit += 1
#   Since we got outside the loop, our coefficient must be␣
 ↪positive.
    print("Coefficient h_%d:" % n)
    show(expand(c))
    print("is positive for p in [8,10].\n\n")
#     print(numit)
```

```
Coefficient h_0:

1/5*(1/8*sqrt(5) + 3/8)^(1/2*p) + 1/5*(-1/8*sqrt(5) + 3/8)^(1/2*p) + 1/3/4^(1/2*p) + 1/60

is positive for p in [8,10].

Coefficient h_1:

-1/200*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 1/200*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
 + 1/40*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 1/40*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
```

```
+ 11/25*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) - 11/25*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 17/50*(1/8*sqrt(5) + 3/8)^(1/2*p) - 17/50*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 1/6*p/4^(1/2*p) + 13/18/4^(1/2*p) + 149/1800
```

is positive for p in [8,10].

Coefficient h_2:

```
9/50*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 9/50*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 11/30*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 11/30*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 44/75*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) - 44/75*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 82/75*(1/8*sqrt(5) + 3/8)^(1/2*p) - 82/75*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 2/3*p/4^(1/2*p) + 14/9/4^(1/2*p) + 59/450
```

is positive for p in [8,10].

Coefficient h_3:

```
14/125*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 14/125*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 6/25*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 6/25*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 8/25*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) - 8/25*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 128/125*(1/8*sqrt(5) + 3/8)^(1/2*p) - 128/125*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 8/15*p/4^(1/2*p) + 104/45/4^(1/2*p) + 154/1125
```

is positive for p in [8,10].

Coefficient h_4:

```
16/875*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 16/875*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
```

```
- 16/175*p*(1/8*sqrt(5) + 3/8)^(1/2*p) - 16/175*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 192/875*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) - 192/875*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 512/875*(1/8*sqrt(5) + 3/8)^(1/2*p) - 512/875*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 64/105/4^(1/2*p) + 272/2625

is positive for p in [8,10].
```

Positivity of h_5, h_7, h_8

Symbolic verification that the last three coefficients turn to 0 at $p = 8$:

[15]:
```
[coeffs[i].subs(p=8).expand() for i in [5,7,8]]
```

[15]:
```
[0, 0, 0]
```

The same applies to h_7 and h_8 at $p = 10$:

[16]:
```
[coeffs[i].subs(p=10).expand() for i in [7,8]]
```

[16]:
```
[0, 0]
```

For h_5 it will suffice to verify that $dh\_5/dp > 0$ on $[8, 10]$. This will be done similarly to the verification of positivity of the coefficients above, using the second derivative $\frac{d^2 h_5}{dp^2}$. For the same reason we shall need 2nd derivatives of h_7, h_8, so we compute them as well.

[17]:
```
coeffs2 = [coeffs[5]] + coeffs[7:9]
```

[18]:
```
deriv2_bounds = []
for c in coeffs2:
    c2prime = diff(diff(expand(c),p),p)
    c2sub = c2prime.subs((1/8*sqrt(5) + 3/8)^(1/2*p)==(1/
↪8*sqrt(5) + 3/8)^(1/2*RIF(8))
              ).subs((-1/8*sqrt(5) + 3/8)^(1/2*p)==(-1/8*sqrt(5)␣
↪+ 3/8)^(1/2*RIF(8))
```

```
                    ).subs(4^(1/2*p)==4^(1/2*RIF(8))
                          ).subs(p=RIF(10))


    deriv2_bound = symbolic_expression(0)
    for o in c2sub.operands():
        deriv2_bound += abs(o)
    deriv2_bounds.append(deriv2_bound.n())
```

[19]:
```
deriv2_bounds
```

[19]:
```
[[0.017230522423253138 .. 0.017230522423253167],
 [0.034153895491620150 .. 0.034153895491620200],
 [0.16177123014881680 .. 0.16177123014881709]]
```

Hence a uniform bound for h_n'', $n = 5, 7, 8$ is e.g. 0.2. Just as above, if for some p_0, $h_n'(p_0) > 0$, then the same applies to $h_n'(p_0 + 5h_n(p_0))$, and also

$$h_n(p) > 0, \qquad p \in [p_0, p_0 + 5h_n(p_0)].$$

We iterate this argument for h_5.

[20]:
```
cprime = diff(expand(coeffs[5]),p)
p_it = RIF(8)
numit = 0
while p_it <= RIF(10):
    p_it = p_it + (5*cprime.subs(p = p_it)).n()
    numit += 1
# print(numit)
print("Derivative of the coefficient h_%d:" % 5)
show(cprime)
```

```
print("is positive for p in [8,10].\n\n")
```

```
Derivative of the coefficient h_5:

16/1575*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)

- 16/1575*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

- 16/315*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)

- 16/315*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

- 128/1575*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)

+ 128/1575*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

+ 64/225*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)

+ 64/225*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

+ 32/1575*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) - 32/1575*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)

- 32/315*(1/8*sqrt(5) + 3/8)^(1/2*p) - 32/315*(-1/8*sqrt(5) + 3/8)^(1/2*p) + 128/189*log(2)/4^(1/2*p)


is positive for p in [8,10].
```

This gives the desired positivity of h_5 on $[8,10]$. To verify positivity of $h_n, n = 7, 8$, we show i) positivity of h'_n on $[8, 8.5]$; ii) negativity of h'_n on $[9.5, 10]$; iii) positivity of h_n on $[8.5, 9.5]$.

[21]:
```
R = RealIntervalField(100)
```

Instead of performing steps with variable length as we did above, we shall make the step size fixed, in order to avoid accumulation of error. To prevent making steps that are too long, the fixed step is compared to $5h'_n(p_0)$. We also increase the precision of interval arithmetic from the default 53 bits to 100 bits.

[22]:
```
for n in (7..8):

    cprime = diff(expand(coeffs[n]),p)

    p_it = R(8)

    step = R(0.00002)
```

```
    numit = 0
    flag = True
    while p_it <= R(8.5):
        if (cprime.subs(p = p_it).n() > step):
            p_it = p_it + 5*step
            numit += 1
        else:
            flag = False
            break
    if (flag):
        print("Derivative of the coefficient h_%d:" % n)
        show(cprime)
        print("is positive for p in [8,8.5].\n\n")
```

```
Derivative of the coefficient h_7:

-64/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 64/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 64/2145*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 64/2145*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 2048/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 2048/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 256/825*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 256/825*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 128/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 128/2145*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/2145*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 512/1287*p*log(2)/4^(1/2*p) + 3584/3861*log(2)/4^(1/2*p) + 512/1287/4^(1/2*p)


is positive for p in [8,8.5].
```

```
Derivative of the coefficient h_8:

-1024/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 1024/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 7168/32175*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 7168/32175*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 32768/160875*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 32768/160875*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 4096/10725*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 4096/10725*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 2048/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 2048/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 14336/32175*(1/8*sqrt(5) + 3/8)^(1/2*p) + 14336/32175*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 8192/19305*p*log(2)/4^(1/2*p) + 8192/4455*log(2)/4^(1/2*p) + 8192/19305/4^(1/2*p)

is positive for p in [8,8.5].
```

Negativity of $h_n'(p)$, for p in $[9.5, 10]$:

[23]:
```
for n in (7..8):
    cprime = diff(expand(coeffs[n]),p)
    p_it = R(9.5)
    step = R(0.00001)
    numit = 0
    flag = True
    while p_it <= R(10):
        if (cprime.subs(p = p_it).n() < -step):
            p_it = p_it + 5*step
            numit += 1
        else:
```

```
            flag = False
            break
    if (flag):
        print("Derivative of the coefficient h_%d:" % n)
        show(cprime)
        print("is negative for p in [9.5,10].\n\n")
```

```
Derivative of the coefficient h_7:

-64/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 64/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 64/2145*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 64/2145*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 2048/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 2048/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 256/825*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 256/825*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 128/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)
+ 128/2145*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/2145*(-1/8*sqrt(5) + 3/8)^(1/2*p)
- 512/1287*p*log(2)/4^(1/2*p) + 3584/3861*log(2)/4^(1/2*p) + 512/1287/4^(1/2*p)


is negative for p in [9.5,10].



Derivative of the coefficient h_8:

-1024/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 1024/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
+ 7168/32175*p*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
+ 7168/32175*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)
- 32768/160875*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)
```

```
+ 32768/160875*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

+ 4096/10725*(1/8*sqrt(5) + 3/8)^(1/2*p)*log(1/8*sqrt(5) + 3/8)

+ 4096/10725*(-1/8*sqrt(5) + 3/8)^(1/2*p)*log(-1/8*sqrt(5) + 3/8)

- 2048/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 2048/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 14336/32175*(1/8*sqrt(5) + 3/8)^(1/2*p) + 14336/32175*(-1/8*sqrt(5) + 3/8)^(1/2*p)

- 8192/19305*p*log(2)/4^(1/2*p) + 8192/4455*log(2)/4^(1/2*p) + 8192/19305/4^(1/2*p)


is negative for p in [9.5,10].
```

It remains to justify positivity of h_n itself in the interval $[8.5, 9.5]$. Since h_n is positive at the endpoints of this interval, the strategy used for the first five coefficients applies here as well.

[24]:
```
for n in (7..8):
    c = expand(coeffs[n])
    p_it = R(8.5)
    step = R(0.00001)
    numit = 0
    flag = True
    while p_it <= R(9.5):
        if (c.subs(p = p_it).n() > step):
            p_it = p_it + step
            numit += 1
        else:
            flag = False
            break
    if(flag):
        print("Coefficient h_%d:" % n)
        show(c)
```

```
        print("is positive for p in [8.5,9.5].\n\n")
```

```
Coefficient h_7:

-128/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 128/2145*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 128/2145*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)

- 4096/10725*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 4096/10725*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 512/825*(1/8*sqrt(5) + 3/8)^(1/2*p) + 512/825*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 512/1287*p/4^(1/2*p) - 3584/3861/4^(1/2*p) - 128/8775


is positive for p in [8.5,9.5].



Coefficient h_8:

-2048/10725*sqrt(5)*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 2048/10725*sqrt(5)*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 14336/32175*p*(1/8*sqrt(5) + 3/8)^(1/2*p) + 14336/32175*p*(-1/8*sqrt(5) + 3/8)^(1/2*p)

- 65536/160875*sqrt(5)*(1/8*sqrt(5) + 3/8)^(1/2*p) + 65536/160875*sqrt(5)*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 8192/10725*(1/8*sqrt(5) + 3/8)^(1/2*p) + 8192/10725*(-1/8*sqrt(5) + 3/8)^(1/2*p)

+ 8192/19305*p/4^(1/2*p) - 8192/4455/4^(1/2*p) - 2048/289575


is positive for p in [8.5,9.5].
```

A.3 Magma code to generate the new weighted projective design

The below magma script constructs a weighted projective 3-design of 85 vectors in $\mathbb{C}^5$, which is absent from recent survey papers on minimal sized cubature formulas. There are two parts of the configuration which take different weights. In the system, 45 vectors arise as the $W(K_5)$ complex reflection group generators. The other 40 vectors, after being embedded into 10-dimensional real space, are minimal vectors of the shorter Coxeter-Todd lattice, also known as O_{10} (see [111]).

The relationship between the two configurations is that the 45 vectors from the $W(K_5)$ reflection group can be realified to obtain vectors which are minimal vectors of the maximal even sublattice of $O_1 0$, $(C6xSU(4,2)) : C2$. The FrameSymmetry program used below to compute the symmetry group of the new configuration is by Grassl and Waldron, and may be found in [74].

First we generate a transformation U.

```
F<w>:=CyclotomicField(6);
R<x>:=PolynomialRing(Integers());
f:=x^2-3;
Q<a>:=ext<F|f>;
U:=1/2*Matrix(Q,5,5,[[1,w^5,w^5,1,0],[-1,1,w^4,0,-w^4],[w^4,0,-w^4,1,1],\
[0,1,-w^5,w^5,-1],[-w^4,-w^5,0,w^5,-w^4]]);
```

We check that U is unitary.

```
S:=ZeroMatrix(F,5,5);
for w in [1 .. 5] do
for u in [1 .. 5] do
S[u,w]:=ComplexConjugate(U[u,w]);
end for;
end for;
U*Transpose(S);
```

Next we build the 45 vector system...

```
T:=Matrix(Q,[[1,0,0,0,0], [0, 1/2, w^2/2, w^2/2, 1/2], [0, 1/2, w^5/2, w^2/2, 1/2],\
 [0, 1/2, w^5/2, w^5/2, 1/2], [0, 1/2, w^5/2, w^5/2,-1/2],\
 [0, 1/2, w^2/2, w^5/2, 1/2], [0, 1/2, w^2/2, w^5/2,-1/2],\
 [0, 1/2, w^5/2, w^2/2,-1/2], [0, 1/2, w^2/2, w^2/2,-1/2],\
 [0,1,0,0,0], [ 1/2,0, 1/2, w^2/2, w^2/2], [ 1/2,0, 1/2, w^5/2, w^2/2],\
 [ 1/2,0, 1/2, w^5/2, w^5/2], [-1/2,0, 1/2, w^5/2, w^5/2],\
 [ 1/2,0, 1/2, w^2/2, w^5/2], [-1/2,0, 1/2, w^2/2, w^5/2],\
 [-1/2,0, 1/2, w^5/2, w^2/2], [-1/2,0, 1/2, w^2/2, w^2/2],\
 [0,0,1,0,0], [ w^2/2, 1/2,0, 1/2, w^2/2], [ w^2/2, 1/2,0, 1/2, w^5/2],\
 [ w^5/2, 1/2,0, 1/2, w^5/2], [ w^5/2,-1/2,0, 1/2, w^5/2],\
 [ w^5/2, 1/2,0, 1/2, w^2/2], [ w^5/2,-1/2,0, 1/2, w^2/2],\
```

```
[ w^2/2,-1/2,0, 1/2, w^5/2], [ w^2/2,-1/2,0, 1/2, w^2/2],\
[0,0,0,1,0], [ w^2/2, w^2/2, 1/2,0, 1/2], [ w^5/2, w^2/2, 1/2,0, 1/2],\
[ w^5/2, w^5/2, 1/2,0, 1/2], [ w^5/2, w^5/2,-1/2,0, 1/2],\
[ w^2/2, w^5/2, 1/2,0, 1/2], [ w^2/2, w^5/2,-1/2,0, 1/2],\
[ w^5/2, w^2/2,-1/2,0, 1/2], [ w^2/2, w^2/2,-1/2,0, 1/2],\
[0,0,0,0,1], [ 1/2, w^2/2, w^2/2, 1/2,0], [ 1/2, w^5/2, w^2/2, 1/2,0],\
[ 1/2, w^5/2, w^5/2, 1/2,0], [ 1/2, w^5/2, w^5/2,-1/2,0],\
[ 1/2, w^2/2, w^5/2, 1/2,0], [ 1/2, w^2/2, w^5/2,-1/2,0],\
[ 1/2, w^5/2, w^2/2,-1/2,0], [ 1/2, w^2/2, w^2/2,-1/2,0]]);
```

and build the 40 vector system

```
W:=Matrix(Q,[[ 1, 0, w^2, w^2, 0, 1, 0, w^2, -w^2, 0,\
 1, 0, -w^2, w^2, 0, 1, 0, -w^2, -w^2, 0,\
 1, 0, 0, 1, w^2, 1, 0, 0, 1, -w^2,\
 1, 0, 0,-1, w^2, 1, 0, 0,-1, -w^2],\
 [ 0, 1, 0, w^2, w^2, 0, 1, 0, w^2, -w^2,\
 0, 1, 0, -w^2, w^2, 0, 1, 0, -w^2, -w^2,\
 w^2, 1, 0, 0, 1, -w^2, 1, 0, 0, 1,\
 w^2, 1, 0, 0,-1, -w^2, 1, 0, 0,-1],\
 [ w^2, 0, 1, 0, w^2, -w^2, 0, 1, 0, w^2,\
 w^2, 0, 1, 0, -w^2, -w^2, 0, 1, 0, -w^2,\
 1, w^2, 1, 0, 0, 1, -w^2, 1, 0, 0,\
-1, w^2, 1, 0, 0,-1, -w^2, 1, 0, 0],\
 [ w^2, w^2, 0, 1, 0, w^2, -w^2, 0, 1, 0,\
 -w^2, w^2, 0, 1, 0, -w^2, -w^2, 0, 1, 0,\
 0, 1, w^2, 1, 0, 0, 1, -w^2, 1, 0,\
 0,-1, w^2, 1, 0, 0,-1, -w^2, 1, 0],\
 [ 0, w^2, w^2, 0, 1, 0, w^2, -w^2, 0, 1,\
 0, -w^2, w^2, 0, 1, 0, -w^2, -w^2, 0, 1,\
 0, 0, 1, w^2, 1, 0, 0, 1, -w^2, 1,\
 0, 0,-1, w^2, 1, 0, 0,-1, -w^2, 1]]);
J:=U*W;
S2:=ZeroMatrix(Q,5,40);
```

```
for r in [1 .. 40] do
for u in [1 .. 5] do
S2[u,r]:=1/a*J[u,r];
end for;
end for;
```

We compute the gram matrix and automorphism group of the compound of the two configurations.

```
H:=HorizontalJoin(Transpose(T),S2);
S3:=ZeroMatrix(Q,5,85);
for r in [1 .. 85] do
for u in [1 .. 5] do
S3[u,r]:=ComplexConjugate(H[u,r]);
end for;
end for;
Attach("FrameSymmetry.m");
Gr:=Transpose(S3)*H;
FrameSymmetry(Gr);
```

We then calculate the permutation group acting on a set of cardinality 85. The order is $25920 = 2^6 \cdot 3^4 \cdot 5$. It can be checked by same procedure that FrameSymmetry applied to either system alone gives a group of order $2 \cdot 25920 = 51840$.

Lastly, we check the weighted design condition

```
s:=0;
for k in [1 .. 45] do
for l in [1 .. 45] do
s:=s+(Gr[k,l]*ComplexConjugate(Gr[k,l]))^3*4/315*4/315;
end for;
end for;
t:=0;
for k in [46 .. 85] do
```

```
for l in [46 .. 85] do
t:=t+(Gr[k,l]*ComplexConjugate(Gr[k,l]))^3*3/280*3/280;
end for;
end for;
q:=0;
for k in [1 .. 45] do
for l in [46 .. 85] do
q:=q+(Gr[k,l]*ComplexConjugate(Gr[k,l]))^3*4/315*3/280;
end for;
end for;
s+t+2*q;
```

This value is $1/\binom{d+t-1}{t} = 1/\binom{7}{3} = 1/35$, the correct value for a weighted 3-design in $\mathbb{CP}^4$.

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